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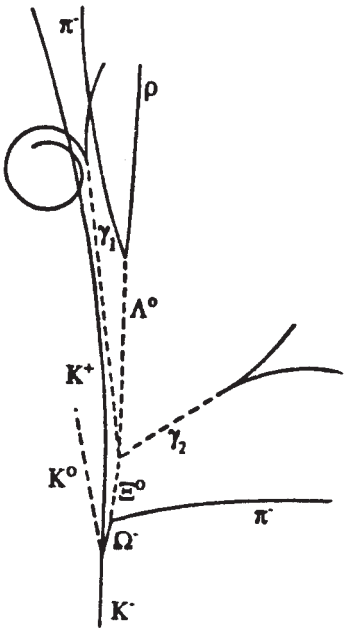

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Phase Shift Analysis in Nuclear Astrophysics and Three-Body Model for Some Nuclei

Part I. Methods of Solution of the Schrödinger Equation, 3-95

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Dubovichenko Sergey Borisovich

Fesenkov Astrophysical Institute – Observatory 23, Kamenskoe plato, 050020, Almaty, Republica of Kazakhstan

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Dubovichenko S.B.

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Introduction

In many problems of the nuclear physics at low energies and nuclear astrophysics the knowledge of the scattering elastic phase shifts, which can be determined from the differential cross sections of scattering of the various nuclear particles is required [1]. Such phase shifts are used, in particular, for construction of the intercluster interaction potentials, for example, in the potential cluster model (PCM) of easy light nuclei [2]. The procedure of the phase shift analysis consists in the decomposition of the total scattering amplitude in a row by the partial waves or amplitudes and the analysis of the parameters appearing at the same time, which are called the scattering phase shifts. Such phase shifts allow one to obtain the data about the nature of strong interactions, the structure of resonance states and the general structure of an atomic nucleus [1].

The two-body processes with the formation of resonances in the nuclear physics at low energies also can be investigated by the means of the phase shift analysis. To solve this problem it is necessary to consider in details the energy behavior of the resonance partial scattering amplitude [1,3]. As a result, the phase shift analysis plays a large role in the search of nuclear resonances of the scattering processes and determination of their quantum numbers. The research of the scattering processes by the means of the phase shift analysis allows one to clarify many important aspects of the interactions of nuclear particles, because this analysis is based only on the most general conservation laws and is closely connected with experimental data [1,3].

The problem of determination or extraction of the nuclear phase shifts from the cross sections of elastic scattering in the mathematical plan is reduced to a multiple parameter variation problem. In other words, when the experimental scattering cross sections of nuclear particles and mathematical expressions obtained in the quantum mechanics, which describe these cross sections depending on some δ_L parameters - nuclear scattering phase shifts are known, there is a multiple parameter variation problem of finding of these parameters on the set interval of values taking into account the generalized Levinson's theorem [4]. In different nuclear systems depending on the energy of the colliding particles, the number of

elastic scattering phase shifts can change from 1–3 to 10–20 [5].

This book is directly based on the results about two tens scientific articles published generally for the last five-seven years in Russia, Europe, USA and the CIS countries and consists of three chapters. The first of them is devoted to the description of the general mathematical methods of calculation of some nuclear characteristics. The general criteria and methods of creation of the intercluster potentials in a continuous and discrete spectrum, which are used further for the consideration of some nuclei in the three-body model described in the third chapter, are defined.

The second chapter contains methods and results of the phase shift analysis of the elastic scattering of the nuclear particles ^{4}He^{4}He, n^{3}He, p^{6}Li, p^{12}C, n^{12}C, p^{13}C, p^{14}C, n^{16}O, p^{16}O and ^{4}He^{12}C at low and astrophysical energies. These results are used for the construction in the PCM of pair intercluster interaction potentials of the continuous spectrum. Here the various experimental measurements, methods of calculations of differential cross sections, computer programs and results of the phase shift analysis of elastic scattering of the particles stated above will be considered. For the first system ^{4}He^{4}He only the main expressions for the phase shift analysis, the computer program and versions of the control account are given at 25–29 MeV. For other systems, except the last, the area of energies approximately to 1–2.5 MeV is considered. In an elastic ^{4}He^{12}C scattering the phase shift analysis is made in the range of 1.5–6.5 MeV. The areas of the phase shift analysis given here are caused by the existence of the experimental data on the differential cross sections for the angular distributions or excitation functions.

The results obtained in the three-body single-channel models of some light nuclear nuclei, namely, ^{7}Li, ^{9}Be and ^{11}B are given in chapter three. They allow one to check the adequacy of the construction pair intercluster potentials on the basis of the elastic scattering phase shifts and characteristics of the bound states of light atomic nuclei. These results allow one to find out the applicability of the obtained potentials in the three-body problems. The potentials checked thus are used further for the calculations of some main characteristics of thermonuclear processes of the preliminary nucleosynthesis of the Universe and some solar cycles [2].

Let us note that the second and, especially, the third chapters of this book almost completely coincide with the results given in the

corresponding chapters of other book of the author: "Preliminary nucleosynthesis of the Universe" of Germany, Saarbrucken: Lambert Academy Publ. GmbH&Co. KG. 2014. 668 pages [2]. This material is selected to the separate book "Phase shift analysis...", primarily in order to reduce book [2] and allows if future the possibility of its enlargement and addition by new material on thermonuclear reactions at the next reedition. At the same time, the present book can also be extended at the inclusion in its new results by the phase shift analysis or three-body model.

I. Methods of Solution of the Schrödinger Equation

Introduction

The set of problems of theoretical nuclear physics, especially in the field of light atomic nuclei and low energies, demands the ability to solve the Schrödinger equation or the coupled system of the equations of this type. Wave function, which describes a quantum state of some system of nuclear particles and, in principle, contains all information about such state is a result of the solution.

There are very many various mathematical methods of the solution of the differential equations or their systems of the second order, which the Schrödinger equation is. However, quite abstract methods of solutions of such equations, which are rather difficult to apply to the solution of the concrete equation, Schrödinger equation type, are usually given in mathematical literature. The problem is usually made by the choice of the most optimum mathematical and numerical method applicable for the consideration of the certain problems based on the solutions of the Schrödinger equation.

This chapter is devoted to the solution of these problems, and describes some of the mathematical methods directly applicable to the location of the wave functions from the Schrödinger equation of scattering problems of nuclear particles and their bound states. The numerical methods of decisions applicable in the problems of a continuous and discrete spectrum of states, which allow one to obtain the end results with almost complete accuracy are considered. On the basis of these methods the possibility of writing of computer programs in the Basic language for the compiler Turbo Basic of Borland and Fortran-90 firm is considered, which really allows one to solve all problems of nuclear physics considered here.

Many problems of nuclear physics can be considered when using only the central part of the nuclear forces [6,7]. In this case there is only one Schrödinger equation or the system of unrelated equations (at the accounting of spin-orbital interaction) and the mathematical problem is

solved rather simply. The account tensor components of nuclear forces leads us to the system of the bound Schrödinger equations [8,9], the solution of which is slightly more difficult, but quite feasible by many methods, including, described in work [10].

We will provide the mathematical and numerical methods used at the solution of the Schrödinger equations for the central potentials at the positive and negative eigenvalues in this chapter. We will consider their application for the analysis of scattering quantum problem and bound state energies of the nuclear particles. In other words, the methods of search of nuclear scattering phase shifts and calculation of the bound states energies of light nuclei within the modified potential two-cluster model (MPCM) [2] are given.

1.1 The general methods of solution of the Schrödinger equation

In this paragraph the general formulation of the problem for the solution of the Schrödinger equation at the positive continuous and negative discrete eigenvalues will be considered. Entry and boundary conditions for solving this problem will be determined, under which such problem is solved, in the relation to the description of the physical processes and states in nuclear physics and nuclear astrophysics.

1.1.1 The central real potentials

The Schrödinger equation for the central forces of interaction between two nuclear particles without spin-orbital and tensor potentials has the following form [1,6,7,11]

$$u''(r)+\left[k^2-V_c(r)-V_{coul}(r)-\frac{L(L+1)}{r^2}\right]u(r)=0\ , \qquad (1.1.1)$$

where r is the scalar relative distance between particles in fm (1 fermi = 10^{-15} m), u – solutions of the equation, i.e., wave functions (WF), u'' – its second derivative, $V_{coul}(r) = 2\mu/\hbar^2\ Z_1Z_2/r$ is the Coulomb potential reduced to the dimension of fm^{-2}, $\hbar$ – Plank constant = 1.055 10^{-34} J s – Joule by second, Z_1 and Z_2 – charges of particles in terms of elementary charge (1 e.c. – elementary charge = 1.60 10^{-19} C – Coulomb), constant $\hbar^2/m_0$ = 41.4686 MeV fm^2 (1 MeV – megaelectronvolt = 1.60 10^{-13} Joule), m_0 – atomic mass unit (1 amu – atomic mass unit = 1.66 10^{-27} kg.), $V_{cf} = L(L+1)/r^2$ – the centrifugal potential, which depends on the value of the orbital moment of the relative movement of the L particles, $k^2 = 2\mu E/\hbar^2$ – wave number of the relative motion in fm^2, E – energy of particles in MeV, $\mu = \frac{m_1m_2}{m_1+m_2}$ – the reduced mass of two particles in amu, $V_c(r)$ – the central part of the nuclear potential, equal to $2\mu/\hbar^2\ V_n(r)$, $V_n(r)$ – the radial dependence of the potential, which is often accepted in a form $V_0\exp(-\alpha r^2)$ or $V_0\exp(-\alpha r)$, V_0 – potential depth in MeV, $\eta = \frac{\mu Z_1Z_2}{\hbar^2 k}$ = 0.0344476 Z_1Z_2/k – the Coulomb parameter and Coulomb potential can be presented in the form

$V_{coul}(r) = 2\eta k/r = A_c/r.$

If the spin-orbital interaction is taken into account, then the central potential has a form [1,6,7]

$V_c(r) = 2\mu/\hbar^2 [V_n(r) + V_{sl}(r)],$

$V_{sl}(r) = (\boldsymbol{SL})\ V_{0sl}\ F(r),$

where $F(r)$ – the functional dependence of the potential on the relative distance between particles, which also can be accepted in the form of Gaussian function $\exp(-\alpha r^2)$ or exponent $\exp(-\alpha r)$.

The ***(SL)*** value is called the spin-orbital operator, and its values can be found from the well-known expression [6,7]

$(\boldsymbol{SL})\ u(r) = 1/2\ [J(J+1) - L(L+1) - S(S+1)]\ u(r),$

where J – the total moment of the system, L – the orbital moment, S – spin of the system of particles. Taking into account the spin-orbital interaction, the Schrödinger equation is splitting to system of uncoupled equations, each of which allows one to find the WF for the concrete total moment.

Sometimes into the potential of interaction the Coulomb R_c radius is entered, and then the Coulomb part of the potential takes a slightly different form

$$V_{coul}(r) = \frac{2\mu}{\hbar^2} \begin{cases} \dfrac{Z_1 Z_2}{r} & r > R_c \\ Z_1 Z_2 \left(3 - \dfrac{r^2}{R_c^2}\right) \Big/ 2R_c & r < R_c \end{cases} \qquad (1.1.2)$$

The equation (1.1.1) forms the Cauchy problem with initial conditions, which get out from the physical reasons. The first initial condition demands the equality to zero of the WF at $u(0) = 0$. As the WF reflects the probability of some processes or states of the quantum particles, this condition means that two particles cannot completely merge and occupy

the same volume. The second statement of the Cauchy problem has to be a determination of the value of the first derivative of this function. But because of the physical reasons, it is impossible to determine the value of this derivative; therefore it is taken equal to some constant, which determines the amplitude of the wave function. In the numerical calculations usually accept $u'(0) = 0.1–1$. The real amplitude of function, which is used for the numerous physical calculations, is defined from the asymptotic conditions imposed on this function at long distances of $r \to R$, when the nuclear potential is almost equal to zero.

The asymptotics of the wave function at long distances, when $V_c(r \to R) \to 0$ is the solution of the equation (1.1.1) without the nuclear potential and can be presented as follows

$$u_L(r \to R) \to F_L(kr) + \mathrm{tg}(\delta_L) G_L(kr) \qquad (1.1.3)$$

or

$$u_L(r \to R) \to \cos(\delta_L) F_L(kr) + \sin(\delta_L) G_L(kr),$$

where F_L and G_L – the scattering Coulomb functions [12,13], which are partial solutions of the equation (1.1.1) without the nuclear part of the potential, i.e., when $V_c = 0$.

Lacing the numerical solution $u(r)$ of equation (1.1.1) at long distances (R about 10–20 fm) with this asymptotics, it is possible to find the real amplitude of the function and the scattering phase shift δ_L for each L at the given energy of the interacting particles. The scattering phase shifts in the concrete system of the nuclear particles can be determined from the phase shift analysis of experimental data by their elastic scattering (chapter 2). Furthermore, the variation of parameters of the nuclear potential in the previously determined form in equation (1.1.1) is carried out and those parameters, which allow one to describe the results of the phase shift analysis are determined. Thus, the problem of the description of scattering processes of nuclear particles consists in search of parameters of the nuclear potential, which describe the results of the phase shift analysis, and, so the experimental data on the scattering cross sections.

We will consider the procedure of lacing of wave functions with their

asymptotics in more detail. At $r = R$ it is possible to write down two equalities for the WF and their derivatives [14]

$$Nu_L(R) = F_L(kR) + \mathrm{tg}(\delta_L)G_L(kR),$$

$$Nu'_L(R) = F'_L(kR) + \mathrm{tg}(\delta_L)G'_L(kR),$$

where N – a normalizing multiplier. It is possible to consider the similar expressions not for the function and derivative, but only for the function in two different points

$$\begin{aligned} Nu_L(R_1) &= F_L(kR_1) + \mathrm{tg}(\delta_L)G_L(kR_1), \\ Nu_L(R_2) &= F_L(kR_2) + \mathrm{tg}(\delta_L)G_L(kR_2). \end{aligned} \qquad (1.1.4)$$

We will enter the notations

$$\begin{aligned} F_1 &= F_L(kR_1), & F_2 &= F_L(kR_2), \\ G_1 &= G_L(kR_1), & G_2 &= G_L(kR_2), \\ u_1 &= u_L(R_1), & u_2 &= u_L(R_2) \end{aligned}$$

and we will find the value N, for example, from the first equation

$$N = [F_1 + \mathrm{tg}(\delta_L)G_1]/u_1.$$

Substituting this expression in the second equation, we will obtain

$$\mathrm{tg}(\delta_L) = (u_1F_2 - u_2F_1)/(u_2G_1 - u_1G_2) = A_L. \qquad (1.1.5)$$

then

$$\delta_L = \mathrm{arctg}(A_L).$$

The function normalization, for our purposes of searching phase shifts, is of no importance. But if we need the normalized WF, i.e., the total

scattering function is also required, then it is better to consider the second equation from (1.1.3), having written down it in the form of (1.1.4) and having performed the similar operations, given above. For the scattering phase shifts turns out the same expression, and the normalization will written in the form

$$N = [\cos(\delta_L)F_1+\sin(\delta_L)G_1]/u_1$$

or

$$N = [\cos(\delta_L)F_2+\sin(\delta_L)G_2]/u_2$$

Thereby, we defines completely the behavior of the wave function, its amplitude and phase shift, in all range of solutions of equation (1.1.1) from zero to some large R, which defines the WF asymptotics.

1.1.2 The central complex potentials

If the inelastic channel of scattering or reactions is open in the nuclear processes, then it is necessary to use the complex potential of interaction, taking into account the decrease of stream of particles from the elastic channel [6]. Now the potential takes a form

$$V_c = V_r(r) + iV_m(r), \qquad (1.1.6)$$

where $V_r(r)$ – the real part of the potential and $V_m(r)$ – its imaginary part. The wave function also becomes complex and can be written in a form

$$u(r) = x(r) + iy(r). \qquad (1.1.7)$$

Then the Schrödinger equation (1.1.1) can be rewritten in the form of the coupled equation system

$$\begin{aligned} x''(r) + [k^2 - V_r(r) - V_{coul}(r) - L(L+1)/r^2]x(r) &= -V_m y(r), \\ y''(r) + [k^2 - V_r(r) - V_{coul}(r) - L(L+1)/r^2]y(r) &= V_m x(r). \end{aligned} \qquad (1.1.8)$$

With the initial conditions of the form

$x(r=0) = 0, \qquad x'(r=0) = \text{const},$
$y(r=0) = 0, \qquad y'(r=0) = \text{const}.$

In the numerical calculations, the value of a constant (const) for derivatives of wave functions also setting at the level of 0.1–1. The asymptotics of wave functions is represented now as follows [6]

$$u(r) = H^{+}(r) + SH^{-}(r) = [F(r) + iG(r)] + S[F(r) - iG(r)], \qquad (1.1.9)$$

where H^{+} – the Hankel function, F and G – the Coulomb functions and S – the scattering matrix, which has a form

$$S = e^{2i\delta} = S_1 + iS_2 = \cos(2\delta) + i\sin(2\delta).$$

At the accounting of inelastic processes the phase shifts of the elastic scattering become complex and are represented as follows

$$\delta = \sigma + i\Delta,$$

where σ and Δ – the real and imaginary part of the phase shift. Then a scattering matrix can be rewritten in a form

$$S = e^{2i\delta} = e^{-2\Delta}e^{2i\sigma} = \eta e^{2i\sigma} = \eta(S_1+iS_2) = \eta[\cos(2\sigma)+i\sin(2\sigma)], \qquad (1.1.10)$$

where $\eta = e^{-2\Delta}$ – inelasticity parameter. For the determination of the scattering phase shifts and parameter of inelasticity we will write down the boundary conditions for the functions in two points in the form of a logarithmic derivative

$$\frac{u_1}{u_2} = \frac{H_1^{+} + SH_1^{-}}{H_2^{+} + SH_2^{-}}, \qquad (1.1.11)$$

where from it is easy to find

$$S = \frac{u_2 H_1^+ - u_1 H_2^+}{u_1 H_2^- - u_2 H_1^-}.$$

Substituting the expressions for the Hankel functions given above (1.1.9) and splitting the real and imaginary part we will obtain

$$S = \frac{C + iD}{A + iB} = K + iM, \qquad (1.1.12)$$

where

$$K = \frac{AC + BD}{A^2 + B^2}, \qquad M = \frac{AD - BC}{A^2 + B^2} \qquad (1.1.13)$$

and

$$A = b - a, \qquad B = -c - d,$$
$$C = a + b, \qquad D = c - d,$$

$$a = x_2 F_1 - x_1 F_2, \qquad b = y_1 G_2 - y_2 G_1,$$
$$c = y_2 F_1 - y_1 F_2, \qquad d = x_1 G_2 - x_2 G_1$$

Thus, all elements of the S matrixes are expressed through the Coulomb functions and solutions of the initial Schrödinger equation (1.1.8) with the given nuclear potential.

Comparing the real and imaginary part of expressions (1.1.10) and (1.1.12) we will obtain

$$S_1 = \cos(2\sigma) = K/\eta,$$
$$S_2 = \sin(2\sigma) = M/\eta. \qquad (1.1.14)$$

and

$$S^2 = \eta^2 (S_1 + S_2)^2 = \eta^2 ,$$

$$S^2 = K^2 + M^2 \ , \tag{1.1.15}$$

where from we find

$$\eta^2 = K^2 + M^2$$

- the inelasticity parameter. Now knowing these values, we will obtain

$$A = \mathrm{tg}(\sigma) = \frac{S_2}{1+S_1}. \tag{1.1.16}$$

then

$$\sigma = \mathrm{arctg}(A). \tag{1.1.17}$$

It is not difficult to check that when $V_m = 0$ and the equations (1.1.8) become independent, then the $\eta = 1$, and results for phase shifts (1.1.5) and (1.1.16) will coincide.

For the determination of the normalization of the WF we use the expressions (1.1.9) and (1.1.7)

$$N(x+iy) = H^{+}(r) + SH^{-}(r) = [F(r) + iG(r)] + (S_1 + iS_2)\,[F(r) - iG(r)].$$

Where from we find

$$N = \frac{Ax+By}{x^2+y^2} + i\frac{Bx-Ay}{x^2+y^2},$$

where

$$A = (1 + S_1)F(r) + S_2G(r), \qquad B = (1 - S_1)G(r) + S_2F(r).$$

Generally, the normalization of the complex WF can be written down in the form of complex value

$Nu(r) = (N_1 + iN_2)(x + iy) = N_1x - N_2y + i[N_1y + N_2x] = v + iw.$

Here v and w are already normalized total wave functions of the scattering. Equating the real and imaginary part, we will have

$$N_1 = \frac{Ax + By}{x^2 + y^2}, \qquad N_2 = \frac{Bx - Ay}{x^2 + y^2}$$

- the general expressions for the determination of a normalization of the scattering WF in case of the complex potentials [15].

1.2 The numerical methods of solution of the Schrödinger equation

For numerical solution of the Schrödinger equation it is possible to use the finite-difference method (FDM) [7], presenting the function and its derivative in the form of the central differences, using the known Runge-Kutt method (RKM) [16] or the Numerov method (NM) [17], which allow one to obtain the higher accuracy of solution of the initial equation.

1.2.1 The central real potentials

We will write down the Schrödinger equation for the central nuclear forces (1.1.1) in the form of [6]

$$u''(r) + [k^2 - V(r)]u(r) = 0. \qquad (1.2.1)$$

To solve it, it is possible to use the finite-difference method, in which the second derivative can be presented as follows [7]

$$u''(r) = [u(r + h) - 2u(r) + u(r - h)]/h^2 = [u(r_{i+1}) - 2u(r_i) + u(r_{i-1})]/h^2, \quad (1.2.2)$$

where h – a step of the finite-difference grid, for determination of which the whole interval of h values from zero to some R, is divided into N parts

$$h = R/N.$$

Here R – the top limit, on which the lacing of the numerical solution of equation (1.2.1) with its asymptotics is carried out. Then

$$r_i = hi, \qquad u_i = u(r_i)$$

where i changes from 0 to N ($r_0 = 0$ and $r_N = R$). Now expression (1.2.2) can be rewritten in a form

$$u'' = [u_{i+1} - 2u_i + u_{i-1}]/h^2,$$

and the whole equation will be rewritten as

$[u_{i+1} - 2u_i + u_{i-1}]/h^2 + [k^2 - V(r_i)]u_i = 0.$

From where we find (the order of accuracy of $O(h^2)$ is equal to h^2, i.e. the method meets in the proportion to a square of a step [7])

$$u_{i+1} = \left[2 + h^2 V(r_i) - h^2 k^2\right] u_i - u_{i-1} + O(h^2). \qquad (1.2.3)$$

Here $i = 1, 2 \ldots N - 1$. The function at $r = 0$ has to be equal to zero, and on the first step can be accepted equal to some constant, which defines only a function normalization, without affecting its behavior at the various r. From here the WF on the following step of u_2 was found and this process repeats until i would not become equal to $N - 1$. Such procedure allows one to find the whole array of WF values in all points from zero to R. Furthermore, we carry out its lacing in two points, for example, at $r_N = R$ and $r_{N-5} = R - 5h$, as it is described in paragraph 1.1.1. The second point is defined experimentally in each case and depends on the energy of particles, but at small energies usually happens to recede enough back by 3–5 steps [18].

We will give an example of the program on Fortran-90, realizing the described method. Here

U – the array of the WF with a dimension of N,
H – the look of the WF,
N – the number of steps,
A0 – the V_0 depth of the central part of potential in fm^{-2},
R0 – the α width of the central part of the potential in fm^{-2},
L – the orbital moment,
RC - the Coulomb radius R_c in fm,
AK – the Coulomb coefficient A_c in the description of the equation (1.1.1),
SK – wave number of k^2 in fm^{-2}.

```
SUBROUTINE FUN(U,H,N,A0,R0,L,RC,AK,SK)
IMPLICIT REAL(8) (A-Z)
INTEGER N,L,K
DIMENSION U(0:N)
```

```
! INITIAL VALUES
U(0)=0.0D0; U(1)=0.1D0; RR=1.0D0/RC
LL=L*(L+1); BB=AK/(2.0D0*RCU); HK=H*H; SHS=SK*HK-2.0D0
! CALCULATION THE VALUES OF THE Vc(R) POTENTIAL
DO K=1,N-1
X=K*H; XX=X*X
V=A0*DEXP(-R0*XX)+LL/XX
IF (X>RC) THEN
V=V+AK/X
ELSE
V=V+(3.0D0-(X*RR)**2)*BB
ENDIF
! CALCULATION THE VALUES OF THE WAVE FUNCTION
Q=V*HK-SHS
U(K+1)=Q*U(K)-U(K-1)
ENDDO
END
```

The WF $u(r)$ is the calculation result at the given L, for the Schrödinger equation (1.2.1) in the range of values from 0 to R.

1.2.2 The central complex potentials

If there is a system of equations (1.1.8) for the complex potential [18]

$$x''(r) + [\, k^2 - V_r(r) - V_{coul}(r) - L(L+1)/r^2 \,]x(r) = - V_m y(r)$$
$$y''(r) + [\, k^2 - V_r(r) - V_{coul}(r) - L(L+1)/r^2 \,]y(r) = V_m x(r) \qquad (1.2.4)$$

then, using the same representation of a derivative in the final-difference look

$$u'' = [u_{i+1} - 2u_i + u_{i-1}]/h^2$$

for functions x and y we will obtain

$$x_{i+1} = [\, 2 - A_i h^2 \,]x_i - x_{i-1} - h^2 V_m(r_i) y_i,$$

(1.2.5)

$$y_{i+1} = [2 - A_i h^2]y_i - y_{i-1} + h^2 V_m(r_i)x_i,$$

where

$$A_i = k^2 - V_r(r_i) - V_{coul}(r_i) - L(L+1)/r_i^2$$

Also setting the values of functions in the two first points

$$x_0 = 0, \qquad x_1 = \text{const}, \qquad y_0 = 0, \qquad y_1 = \text{const}$$

it is possible to find the values of functions in all other points [18], as well as in case of expression (1.2.3). The lacing procedure of the numerical function with its own asymptotics in the case of complex potentials is described in the paragraph 1.1.2.

1.2.3 The Runge-Kutt method for the central real potentials

Now we will consider the other method of the solution of such equations, which is called the Runge-Kutt method of the fourth by step of the h order [16,19,20,21,22]. The standard method of the solution of one differential equation of the first order

$$y' = f(x,y) \tag{1.2.6}$$

with an initial condition

$$y(x_0) = y_0$$

consists in the presentation of the solution on an interval from 0 to some R in the form

$$y_{n+1} = y_n + \Delta y_n, \tag{1.2.7}$$

where n can change from 0 to N ($R = x_N = hN$), h - a solution step, and Δy_n is obtained from the expression

$$\Delta y_n = 1/6(k_1 + 2k_2 + 2k_3 + k_4), \qquad (1.2.8)$$

where

$$k_1 = hf(x_n,y_n), \qquad k_2 = hf(x_n+h/2,\ y_n+k_1/2),$$
$$k_3 = hf(x_n+h/2,\ y_n+k_2/2), \qquad k_4 = hf(x_n+h,\ y_n+k_3).$$

In the case of system of two differential equations of the first order [16-22]

$$y' = f(x,y,z),$$
$$z' = g(x,y,z) \qquad (1.2.9)$$

with initial conditions

$$y(x_0) = y_0, \qquad z(x_0) = z_0$$

the solutions are found from the expressions

$$y_{n+1} = y_n + \Delta y_n,$$
$$z_{n+1} = z_n + \Delta z_n, \qquad (1.2.10)$$

where

$$\Delta y_n = 1/6(k_1 + 2k_2 + 2k_3 + k_4),$$
$$\Delta z_n = 1/6(m_1 + 2m_2 + 2m_3 + m_4) \qquad (1.2.11)$$

and

$$k_1 = hf(x_n,y_n,z_n), \qquad m_1 = hg(x_n,y_n,z_n),$$
$$k_2 = hf(x_n+h/2,\ y_n+k_1/2,\ z_n+m_1/2), \qquad m_2 = hg(x_n+h/2,\ y_n+k_1/2,\ z_n+m_1/2),$$
$$k_3 = hf(x_n+h/2,\ y_n+k_2/2,\ z_n+m_2/2), \qquad m_3 = hg(x_n+h/2,\ y_n+k_2/2,\ z_n+m_2/2),$$
$$k_4 = hf(x_n+h,\ y_n+k_3,\ z_n+m_3), \qquad m_4 = hg(x_n+h,\ y_n+k_3,\ z_n+m_3).$$

In the case of one differential equation of the second order of the form

(1.2.1)

$$y'' = g(x,y,y') \qquad (1.2.12)$$

with initial conditions

$$y(0) = y_0, \qquad y'(0) = y'_0$$

we use the substituting

$$z = y'.$$

Then we obtain the system of the form

$$\begin{aligned} y' &= z, \\ z' &= g(x,y,z) \end{aligned} \qquad (1.2.13)$$

with initial conditions

$$y(0) = y_0, \qquad z(0) = z_0$$

the solution of which at $f(x,y,z) = z$ can be presented as follows

$$\begin{aligned} \Delta y_n &= hz_n + 1/6h(m_1 + m_2 + m_3), \\ \Delta z_n &= 1/6(m_1 + 2m_2 + 2m_3 + m_4) \end{aligned} \qquad (1.2.14)$$

and

$$\begin{aligned} k_1 &= hz_n, & m_1 &= hg(x_n,y_n,z_n) \ , \\ k_2 &= h(z_n+m_1/2), & m_2 &= hg(x_n+h/2, y_n+k_1/2, z_n+m_1/2) \ , \\ k_3 &= h(z_n+m_2/2), & m_3 &= hg(x_n+h/2, y_n+k_2/2, z_n+m_2/2) \ , \\ k_4 &= h(z_n+m_3), & m_4 &= hg(x_n+h, y_n+k_3, z_n+m_3) \ . \end{aligned}$$

The error of the Runge-Kutt method makes an order of $O(h^4)$ and is

higher than in the previous case for the FDM.

We will give an example of the program on the Fortran-90 realizing the described method. Here

U – array of the WF with the dimension of N,
H – the look of the WF,
N – the number of steps,
A0 – the V_0 depth of the central part of the potential in fm^{-2},
R0 – the α width of the central part of potential in fm^{-2},
L – the orbital moment,
RC – the Coulomb radius R_c in fm,
AK – the Coulomb coefficient A_c in the description of equation (1.1.1),
SK – the wave number k^2 in fm^{-2}.

```
SUBROUTINE FUNRK(U,H,N,A0,R0,L,RC,AK,SK)
IMPLICIT REAL(8) (A-Z)
INTEGER I,N,L
DIMENSION U(0:N)
! THE SOLUTION OF THE SCHRÖDINGER EQUATION BY RUNGE-
KUTT METHOD IN ALL AREA OF VARIABLES
VA1=0.0D0;! VA1 - the value of function in zero
PA1=1.0D-1;! PA1 - Value of a derivative in zero
DO I=0,N-1
X=H*I+1.0D-15
CALL RRUN(VB1,PB1,VA1,PA1,H,X,L,SK,A0,R0)
VA1=VB1; PA1=PB1; U(I+1)=VA1
ENDDO
END

SUBROUTINE RRUN(VB1,PB1,VA1,PA1,H,X,L,SK,A0,R0)
IMPLICIT REAL(8) (A-Z)
INTEGER L
! THE SOLUTION OF THE SCHRÖDINGER EQUATION BY THE
RUNGE-KUTT METHOD BY ONE STEP
X0=X; Y1=VA1
CALL FA(X0,Y1,FK1,L,SK,A0,R0)
```

```
FK1=FK1*H; FM1=H*PA1
X0=X+H/2.0D0; Y2=VA1+FM1/2.0D0
CALL FA(X0,Y2,FK2,L,SK,A0,R0,A1,R1)
FK2=FK2*H; FM2=H*(PA1+FK1/2.0D0); Y3=VA1+FM2/2.0D0
CALL FA(X0,Y3,FK3,L,SK,A0,R0,A1,R1)
FK3=FK3*H; FM3=H*(PA1+FK2/2.0D0); X0=X+H; Y4=VA1+FM3
CALL FA(X0,Y4,FK4,L,SK,A0,R0,A1,R1)
FK4=FK4*H; FM4=H*(PA1+FK3)
PB1=PA1+(FK1+2.0D0*FK2+2.0D0*FK3+FK4)/6.0D0
VB1=VA1+(FM1+2.0D0*FM2+2.0D0*FM3+FM4)/6.0D0
END

SUBROUTINE FA(X,Y,FF,L,SK,A0,R0)
IMPLICIT REAL(8) (A-Z)
INTEGER L,L1
! CALCULATION F (X,Y) FUNCTION IN THE RUNGE–KUTT METHOD
VC=A0*DEXP(-R0*X*X)+A1*DEXP(-R1*X*X)
IF (X>RC) GOTO 1
VK=(3.0D0-(X/RC)**2)*AK/(2.0D0*RCU)
GOTO 2
1 VK=AK/X
2 FF=-(SK-VK-VC-L*(L+1)/(X*X))*Y
END
```

The result of the calculation is the wave function $u(r)$ at the given L, which is the solution of the Schrödinger equation (1.2.1) in the range of values from 0 to R.

1.2.4 Calculation of the wave functions by the Numerov method

Still we have the Schrödinger equation in a general form

$$u''(r) + a(r)u(r) = 0,$$

where

$$a(r) = \left[k^2 - V_c(r)\right],$$

$$V_c(r) = 2\mu/\hbar^2 V_n(r) + 2\mu/\hbar^2 \frac{Z_1 Z_2}{r} + \frac{L(L+1)}{r^2},$$

$$V_n(r) = -V_0 \exp(-\alpha r^2)$$

Here V_0 – the potential depth parameter in MeV, and α – the parameter of its width in fm^{-2}.

Then the WF in the Numerov method [17] at the given energy can be found from the expression

$$u_{n+1} = \frac{\left(2 - \frac{5}{6}h^2 a_n\right)u_n - \left(1 + \frac{1}{12}h^2 a_{n-1}\right)u_{n-1}}{1 + \frac{1}{12}h^2 a_{n+1}} + O(h^6).$$

This method allows to find the WF with a convergence rate of $O(h^4)$ [17], that even more than Runge-Kutt method, having the convergence of $O(h^4)$. Here still

$u_{n-1} = u(r_{n-1})$, $r_{n-1} = (n-1)h$, $h = R/N$,
where R – the top limit of integration of the equation, N – number of steps of integration and h – the value of step, n = 1 ... N - 1 and

$u(0) = 0$, $u(1) = \text{const}$.

We will give an example of the program written on the Fortran-90, realizing the described method. Here

U – array of the WF with the dimension of N,
H – the look of the WF,
N – the number of steps,
A0 – the V_0 depth of the central part of the potential in fm^{-2},

R0 – the α width of the central part of potential in fm^{-2},
L – the orbital moment,
RC – the Coulomb radius R_c in fm,
AK – the Coulomb coefficient A_c in the description of the equation (1.1.1),
SK – the wave number of k^2 in fm^{-2}.

```
SUBROUTINE FUN(U,H,N,A0,R0,L,RC,AK,SK)
IMPLICIT REAL(8) (A-Z)
INTEGER N,L,I
DIMENSION U(0:N),V(0:N)
! INITIAL VALUES
U(0)=0.0D0; U(1)=0.1D0; Q0=0.0D0; RR=1/RC; HK=H*H; SHS=SK*HK
LL=L*(L+1); BB=AK/(2.0D0*RC); AA=1.0D0/12.0D0; DD=5.0D0/6.0D0
! CALCULATION OF VALUES FOR THE Vc(r) POTENTIAL
DO I=1,N-1,2
X=I*H; XX=X*X; XP=(I+1)*H; XXP=XP*XP
V(I)=A0*DEXP(-R0*XX) +LL/XX
V(I+1)=A0*DEXP(-R0*XXP)+LL/XXP
IF (X>RC) THEN
V(I)=V(I)+AK/X
V(I+1)=V(I+1)+AK/XP
ELSE
V(I)=V(I)+(3.0D0-(X*RR)**2)*BB
V(I+1)=V(I+1)+(3.0D0-(XP*RR)**2)*BB
ENDIF
ENDDO
! CALCULATION OF VALUES FOR THE WAVE FUNCTION
DO I=1,N-1,1
Q1=SHS-V(I)*HK; Q2=SHS-V(I+1)*HK; B=(1.0D0+AA*Q2)
U(I+1)=((2.0D0-DD*Q1)*U(I)-(1.0D0+AA*Q0)*U(I-1))/B; Q0=Q1
ENDDO
END
```

As a result there is the WF $u(r)$ at the given L, which is the solution of the Schrödinger equation (1.2.1) in the range of values from 0 to R.

1.2.5 Methods of calculation of the binding energy of two-body system

Phase shifts can be used for the construction not only of the scattering potentials, but also the bound states (BS) – ground (GS) or excited (ES) states. Therefore, we will give two methods for calculation of the binding energy of the two-body nuclear system. Such situation takes place, for example, in the S wave of the $^4He^2H$ system of ^6Li, when originally the BS potential is constructed by the corresponding phase shift, and then its parameters are specified according to value of the binding energy, mean square radius and the asymptotic constant (AC) [23].

1.2.5.1 Finite-difference method

The first of them is based on the finite-difference method, which is in detail described in [7,10]. Here we will give briefly these methods of searching the binding energy and the WF for the bound states and scattering processes. The Schrödinger equation [7] for the central potentials

$$u'' + [k^2 - V(r)]\, u = 0$$

with this or that boundary condition at $k^2 < 0$ forms the boundary value problem of the Sturm-Liouville type with boundary conditions

$$u(r = 0) = u_0 = 0,$$
$$u'(r = R)/u(r = R) = u'_N/ u_N = f(\eta, L, Z_N),$$

where f – logarithmic derivative, η – the Coulomb parameter, $Z_N = 2kr_N$, n = 1,2.... N – number of steps, $r_N = R$ – the upper bound of an interval of integration of the equation and at the transition to the second derivative to final differences [24,25,26]

$$u'' = [u_{n+1} - 2u_n + u_{n-1}]/h^2$$

turns into the determined system of the linear algebraic equations

$$u_{n+1} + [h^2k^2 - h^2V(r) - 2]u_n + u_{n-1} = 0$$

The condition of equality to zero of its D_N determinant

$$D_N = \begin{pmatrix} \theta_1 & 1 & 0 & . & . & . & 0 \\ \alpha_2 & \theta_2 & 1 & 0 & . & . & 0 \\ 0 & \alpha_3 & \theta_3 & 1 & 0 & . & 0 \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ 0 & . & 0 & 0 & \alpha_{N-1} & \theta_{N-1} & 1 \\ 0 & . & 0 & 0 & 0 & \alpha_N & \theta_N \end{pmatrix} = 0,$$

allows one to define eigen binding energy of the system of two particles of k_0.

Here N – number of equations, $h = R/N$ –step of the finite-difference grid, R – an interval of the solution of the equation, for example, from zero to 30 fm, and

$$\alpha_n = 1, \qquad \alpha_N = 2, \qquad \theta_n = k^2h^2 - V_nh^2 - 2,$$

$$\theta_N = k^2h^2 - V_Nh^2 - 2 + 2hf(\eta,L,Z_N), \qquad Z_N = 2kr_N,$$

$$r_n = nh, \qquad n = 1,2 \ldots..N, \qquad k = \sqrt{|k^2|},$$

$$f(\eta,L,Z_n) = -k - \frac{2k\eta}{Z_n} - \frac{2k(L-\eta)}{Z_n^2},$$

where $V_n = V(r_n)$ – the potential of the interaction of clusters in r_n point. Such form of record of the boundary conditions in the form of the logarithmic derivative $f(\eta,L,Z_n)$ allows one to consider the Coulomb interaction, i.e. effects, which gives the consideration in an asymptotics of the WF of the Whittaker function for the BS.

The type of the logarithmic derivative of the wave function of the bound state in the external area can be obtained from the integrated representation of the Whittaker function [27]

$$f(\eta, L, Z) = -k - \frac{2k\eta}{Z} - \frac{2k(L-\eta)}{Z^2} S,$$

where

$$S = \frac{\int_0^\infty t^{L+\eta+1}(1+t/z)^{L-\eta-1} e^{-t} dt}{\int_0^\infty t^{L+\eta}(1+t/z)^{L-\eta} e^{-t} dt}.$$

The calculations show that the S value does not exceed 1.05, and its influence on the binding energy of two-body system is negligible.

The calculation of a determinant of D_N is carried out on recurrent formulas of the form

$$D_{-1} = 0, \quad D_0 = 1,$$

$$D_n = \theta_n D_{n-1} - \alpha_n D_{n-2}, \qquad (1.2.15)$$

$$n = 1 \ldots N.$$

For finding the form of wave functions of the bound states other recurrent process is used

$$u_0 = 0, \qquad u_1 = \text{const},$$

$$u_n = -\theta_{n-1} u_{n-1} - u_{n-2}, \qquad (1.2.16)$$

$$n = 2 \ldots N,$$

where const – any number, this is usually setting in the 0.01–0.1 range.

Thereby, at the given energy of the system it is possible to find determinant and wave function of the bound state. The energy leading to the zero determinants

$$D_N(k_0) = 0$$

it considers of the eigen energy of system, and the wave function at this energy is the eigenfunctions of the problem.

The last recurrence relation is used also for the search of the WF in case of a continuous spectrum of eigenvalues, i.e. at the previously given energy ($k^2 > 0$) of scattering particles [10]. The text of the computer program written in the Fortran-90 language is given in work [28].

1.2.5.2 Variation method

The second search method of the binding energy is based on the variation decomposition of the wave function by the non-orthogonal Gaussian basis (VM). We will stop briefly on the description of this method, and the computer program on the Fortran-90 is provided in the book [28]. More detailed statement of this attachment can be found in work [10]. The wave functions in matrix elements for the ground and resonance states are presentable in the form of the decomposition by the non-orthogonal Gaussian basis of the form

$$\Phi_L(r) = \frac{\chi_L(r)}{r} = r^L \sum_i C_i \exp(-\beta_i r^2).$$

which are found by the variation method for the bound states or by the approximation of Gaussian functions of the numerical wave functions of resonance levels [29].

For the determination of the spectrum of eigen energies and wave functions in the standard variation method at decomposition of the WF on the orthogonal basis the matrix problem on the eigenvalues is solved [30]

$$\sum_i (H_{ij} - EI_{ij}) C_i = 0 ,$$

where H – a symmetric matrix of a Hamiltonian, I – a unity matrix, E – eigenvalues and C – eigen vectors of the problem.

In this case, at the non-orthogonal basis the Gaussian functions, we come to the generalized matrix problem of the form [31]

$$\sum_i (H_{ij} - EL_{ij})C_i = 0 \ ,$$

where L – matrix of overlap integrals, which in use the orthogonal basis turns into a unity matrix I.

In use of the WF of the form given above it is easily possible to find the expressions for all two-body matrix elements [31]

$$H_{ij} = T_{ij} + V_{ij} + \left\langle j \left| \frac{Z_1 Z_2}{r} \right| i \right\rangle + \left\langle j \left| \frac{\hbar^2 L(L+1)}{2\mu r^2} \right| i \right\rangle,$$

$$N_0 = \left[\sum C_i C_j L_{ij} \right]^{-1/2},$$

$$T_{ij} = -\frac{\hbar^2}{2\mu} \frac{\sqrt{\pi}(2L-1)!!}{2^{L+1}\beta_{ij}^{L+1/2}} \left\{ L(2L+1) - L^2 - \frac{\beta_i \beta_j (2L+1)(2L+3)}{\beta_{ij}^2} \right\},$$

$$V_{ij} = \int V(r) r^{2L+2} \exp(-\beta_{ij} r^2),$$

$$L_{ij} = \frac{\sqrt{\pi}(2L+1)!!}{2^{L+2}\beta_{ij}^{L+3/2}},$$

$$\left\langle j \left| \frac{Z_1 Z_2}{r} \right| i \right\rangle = \frac{Z_1 Z_2 \, L!}{2\beta_{ij}^{L+1}},$$

$$\left\langle j \left| \frac{\hbar^2 L(L+1)}{2\mu r^2} \right| i \right\rangle = \frac{\sqrt{\pi}(2L-1)!!}{2^{L+1}\beta_{ij}^{L+1/2}} \frac{L(L+1)\hbar^2}{2\mu},$$

$\beta_{ij} = \beta_i + \beta_j$.

In case of the Gaussian potential of intercluster interaction the matrix element of the V_{ij} potential is defined in the analytical form

$$V_{ij} = V_0 \frac{\sqrt{\pi}(2L+1)!!}{2^{L+2}(\beta_{ij} + \alpha)^{L+3/2}},$$

where V_0 and α – the parameter of depth and width of the potential.

1.2.5.3 Method of the solution of generalized matrix problem

And now we will stop briefly on solution methods of the generalized matrix problem [2]. By the consideration of the generalized matrix problem on eigenvalues and eigenfunctions, which turns out after the decomposition of the WF on the non-orthogonal Gaussian basis, we proceed from the standard Schrödinger equation in a general form [32]

$$H\chi = E\chi,$$

where H – Hamiltonian, E – energy of the system and χ – wave functions.

Expand in a series the WF on the non-orthogonal variation basis

$$\chi = \sum_i C_i \varphi_i ,$$

setting up them to the initial system, multiplying it from the left by in a complex interfaced basic function φ_i^* and integrating by all variables, we will obtain the known matrix system of the form [33]

$$(H - EL)C = 0,$$

this generally is the generalized matrix problem for finding of eigenvalues and eigenfunctions [34,35]. If the decomposition of the WF is carried out by the orthogonal basis, the matrix of overlap integrals L turns into a unity matrix of I, and we have a standard problem on eigenvalues, for the solution of which there is a set of methods [36].

For solution of the generalized matrix problem there are also the known methods, given, for example, in the book [16]. In the beginning, we will stop on a standard method of the solution of the generalized matrix problem for the Schrödinger equation, which arises in use of the non-orthogonal variation basis in the nuclear physics or nuclear astrophysics. Then we will consider its modification or an alternative method, which is convenient for applying to the solution of this problem at the numerical

calculations on the modern computers [34].

So, for the determination of the spectrum of eigenvalues of energy and own wave functions in a variation method, at the decomposition of the WF on non-orthogonal Gaussian basis, the generalized matrix problem on eigenvalues [16] is solved

$$\sum_i (H_{ij} - EL_{ij})C_i = 0 \,, \qquad (1.2.17)$$

where H – symmetric matrix of a Hamiltonian, L – matrix of overlap integrals, E – eigenvalues of energy and C – eigen vectors of the problem.

Presenting matrix L in the form of the multiplication of the lower N and the top V triangular matrixes [35], after the simple transformations we pass to usual eigenvalue problem

$$H'C' = EIC',$$

or

$$(H' - EI)C' = 0,$$

where

$$H' = N^{-1}HV^{-1}, \qquad C' = VC,$$

and V^{-1} and N^{-1} the matrices inverse relative to V and N matrices.

Furthermore, we find the matrices of N and V, carrying out a triangularization of symmetric L matrix [36], for example, by the Khaletsky method [35]. Then we determine the matrices inverse N^{-1} and V^{-1}, for example, by the Gauss method and we calculate the matrix elements $H' = N^{-1}HV^{-1}$. Furthermore, we find the total diagonal by E matrix $(H' - EI)$ and we calculate its determinant $\det(H' - EI)$ at some energy E.

Energy, which leads to zero determinant is eigen energy of the problem, and corresponding to its C' vectors are eigen vectors of the orthogonal equation. Knowing C', it is not difficult to find eigen vectors of the initial problem C (1.2.17), because the matrix V^{-1} is already known. The described method of the data of the generalized matrix problem to usual matrix

problem on eigenvalues and functions is called an orthogonalization method according to Schmidt [27]. However, in some problems at some values of the variation parameters the procedure of finding of the matrices inverse is unstable and during the work of the computer program overflow is given.

Therefore, we will consider an alternative method of the numerical solution of the generalized matrix problem on eigenvalues, free from the specified difficulties and having higher speed of the count rate on the computer. Namely, the initial matrix equation (1.2.17) is the homogeneous system of linear equations – it has the nontrivial solutions, only if its determinant det(H - EL) is equal to zero. For the numerical methods realized on the computer it is not obligatory to decompose matrix L to the triangular matrices and to find a new H' matrix and new C 'vector, defining the matrices inverse as it has been described above in use of a standard method.

It is possible to decompose at once the non-diagonal, symmetric matrix *(H - EL)* on the triangular and by the numerical methods in the set area of values to look for the energies, which lead to zero of its determinant, i.e. they are eigen energies. In a real physical problem usually it is not required to look for all eigenvalues and eigenfunctions. It is necessary to find only 1–2 of eigenvalues for certain energy of system and, as a rule, it is the lowest values and eigen wave functions corresponding to them.

Therefore, for example, by the Khaletsky method the initial *(H - EL)* matrix decomposes in to two triangular, and in the main diagonal of the top triangular V matrix there are units

$$A = H - EL = NV$$

and further its determinant at the condition of det(V) = 1 [35] is calculated

$$D(E) = \det(A) = \det(N)\cdot\det(V) = \det(N) = \prod_{i=1}^{m} n_{ii}$$

by zero, by which the necessary eigen value E, i.e. value of energy is looked for. Here m – dimension of matrices, and a determinant of the triangular N matrix is equal to production of its diagonal elements [35].

Thus, we have quite simple problem of search of zero functionality of one variable

$$D(E) = 0,$$

which numerical solution does not represent a big complexity and can be executed with any accuracy, for example, by the bisection method [37].

As a result, we get rid of need to look for two matrices inverse V and N and to carry out the several matrix multiplications to obtain in the beginning a new H' matrix, and then, a final matrix of eigen vectors C. Lack of such operations, especially search of the matrices inverse, considerably increases the account speed on the computer irrespective of a programming language, in which the solution of this problem is realized.

It is possible to use the concept of the residuals [16] for estimation the accuracy of the solution, i.e. the accuracy of the decomposition of an initial matrix to two triangular. After the decomposition of a matrix A to the triangular, the matrix of residuals [16] is calculated as a difference of initial matrix A and a matrix

$$S = NV,$$

where N and V - the found numerical triangular matrices. The difference on all elements with an initial A matrix is calculated

$$A_N = S - A.$$

The A_N matrix of residuals gives a deviation of the approximate NV value found by the numerical methods from true value of each element of an initial A matrix. It is possible to carry out the summation of all elements of the A_N matrix and to obtain the numerical value of the residual. In all variational calculations given here the method which is described above was used, and the maximum value of any element of the A_N matrix usually did not exceed the 10^{-10} value.

The stated method, which is represented quite obvious in the numerical execution allows one to obtain a good stability of the algorithm of the solution of any considered physical problems and does not lead to the

overflow during the work of the computer programs [38]. Thus, the described alternative method of the finding of eigenvalues of the generalized matrix problem [10] considered on the basis of variation methods of the solution of the Schrödinger equation with use of the non-orthogonal variation basis relieves us from the non stability arising together with the application of usual methods of the solution of such mathematical problem, i.e. usual method of orthogonalization by Schmidt.

1.2.6 Methods of calculation of the Coulomb phase shifts

For the practical calculations of the characteristics of the nuclear reactions and scattering processes in many cases, it is necessary to know and, as a rule, with the high precision, the numerical values of the Coulomb functions in the given point R and Coulomb phase shifts in the wide range of values of the Coulomb parameter η. Now many various numerical methods applicable for the finding of these values are known, however, rather recently there were rather simple and reliable representations for the Coulomb functions, and the known ways of calculation of the Coulomb phase shifts possess the number of shortcomings so at their use it is necessary to observe a certain caution.

The Coulomb phase shifts are defined through the G - function as follows [6,39]

$$\sigma_L = \arg\{\Gamma(L+1+i\eta)\}$$

and satisfy to recurrent process $\sigma_L = \sigma_{L-1} + \mathrm{arctg}\left(\frac{\eta}{L}\right)$, where $\eta = \frac{\mu Z_1 Z_2}{\hbar^2 k}$ – the Coulomb parameter, μ – the reduced mass of two particles, k – wave number of the relative movement and $k^2 = 2\mu E/\hbar^2$, E – energy of the colliding particles in the center of masses.

Where from at once it is possible to obtain the following obvious expression

$$\alpha_L = \sigma_L - \sigma_0 = \sum_{n=1}^{L} \mathrm{arctg}\left(\frac{\eta}{n}\right), \qquad \alpha_0 = 0. \tag{1.2.18}$$

The most natural impression for the Coulomb phase shifts is gained on the basis of an integrated formula for the Γ – function [39,52]

$\sigma_L = \mathrm{arctg}(y/x)$,

where

$$y = \int_0^\infty \exp(-t)t^L sin(\eta \ln t)dt$$
$$x = \int_0^\infty \exp(-t)t^L cos(\eta \ln t)dt \quad , \qquad (1.2.19)$$

However, the direct calculation of these integrals appears rather complex problem because subintegral functions are quickly oscillating at $t \to 0$. Therefore, different approximations and asymptotic decomposition, for example, such as representation of the phase shift at $L = 0$ are often used in the form of [41]

$$\sigma_0 = -\eta + \frac{\eta}{2}\ln(\eta^2+16) + \frac{7}{2}\mathrm{arctg}(\eta/4) - [\mathrm{arctg}\eta + \mathrm{arctg}(\eta/2) + \mathrm{arctg}(\eta/3)] -$$

$$-\frac{\eta}{12(\eta^2+16)}[1 + \frac{1}{30}\frac{\eta^2-48}{(\eta^2+16)^2} + \frac{1}{105}\frac{\eta^4-160\eta^2+1280}{(\eta^2+16)^4} + ...]$$

or for the $L >> 1$ [6]

$$\sigma_L = \alpha(L+1/2) + \eta(\ln\beta - 1) + \frac{1}{\beta}\left(-\frac{\sin\alpha}{12} + \frac{\sin 3\alpha}{360\beta^2} - \frac{\sin 5\alpha}{1260\beta^4} + \frac{\sin 7\alpha}{1680\eta^6} - ...\right)$$

where

$$\alpha = \mathrm{arctg}\left(\frac{\eta}{L+1}\right) \quad , \quad \beta = \sqrt{\eta^2 + (L+1)^2} \quad .$$

Using these formulae, all other phase shifts are defined from the recurrent relations (1.2.18). Though both representations have the high speed of the account on the computer, the phase shifts turn out with some error, which can only be estimated having compared the obtained result with the tabular data or calculations on the exact formulae. Besides, the last formula is right only at $L \approx 100$ and the recurrent process gives an additional error in the value of the phase shifts.

Other representations of the Coulomb phase shifts also are known, in particular, at $\eta >> 1$ [42]

$$\sigma_0 = \frac{\pi}{4} + \eta(\log\eta - 1) - \sum_{s=1}^{\infty} \frac{B_s}{2s(2s-1)\eta^{2s-1}} \quad , \qquad (1.2.20)$$

where B_s – the Bernoulli numbers [39]. However, the similar decomposition works well only at $\eta \approx 100$. In works [41,42] it has been shown that it is possible to obtain eight true signs taking into account only the first member of the sum (1.2.20) only at $\eta = 85$. At small η a row converges badly and demands setting or calculation of the Bernoulli numbers.

In work [41] there is other determination of the Coulomb phase shifts

$$\sigma_L = \eta\Psi(L+1) + \sum_{n=1}^{\infty}\left[\frac{\eta}{L+n} - \mathrm{arctg}\left(\frac{\eta}{L+n}\right)\right] \quad , \qquad (1.2.21)$$

which can be obtained from the known form of record Γ-function [39]

$$\Gamma(z) = \Gamma(x+iy) = r\exp(i\phi) = r(\cos\phi + i\sin\phi) \quad ,$$

where

$$\varphi = y\Psi(x) + \sum_{n=0}^{\infty}(\mathrm{tg}\omega_n - \omega_n) \quad , \qquad \omega_n = \mathrm{arctg}\left(\frac{y}{x+n}\right) \quad ,$$

and $\Psi(x)$ – a logarithmic derivative of the Γ– function [39], which for the whole argument has the form

$\Psi(L+1) = -C + 1 + 1/2 + ... + 1/L$.

Here C = 0.5772156649..... – the Euler's constant [39]. Such series will congregate quicker, when the η is less and L is more. This formula covers the area opposite to the representation (1.2.20) and at $1 < \eta < 50$ both decompositions have the bad convergence.

To estimate the remainder term of series (1.2.21) we will decompose an arctangent in a series at $\eta/n << 1$, that is always possible at big n or small η. Then we will obtain

$$\sigma_0 = -C\eta + \sum_{n=1}^{\infty}\left(\frac{\eta^3}{3n^3} - \frac{\eta^5}{5n^5} + \frac{\eta^7}{7n^7} - ...\right) \quad . \tag{1.2.22}$$

From here it is clear that the remainder of series will have an order of the value η^3/n^2 [16]. A series (1.2.22) at $\eta > 1$ congregate rather badly as for obtaining, for example, relative accuracy of 10^{-8} is required to take into account the tens of thousands terms of this series.

However, such row allows the significant improvement of the convergence at $\eta \approx 1$ [50] after the transformation it to the form

$$\sigma_0 = -\eta C + \frac{1}{3}\eta^3 S + \sum_{n=1}^{\infty}\left[\frac{\eta}{n} - \mathrm{arctg}\left(\frac{\eta}{n}\right) - \frac{1}{3}\frac{\eta^3}{n^3}\right] , \tag{1.2.23}$$

where $S = \sum_{k=1}^{\infty}\frac{1}{k^3} = 1.202056903...$. It is simple to find that the residual term of such series is equal to η^5/n^4 and for obtaining eight true signs it is necessary to consider only a few hundreds of members at $\eta \approx 1$.

The series (1.2.23) given above allows additional improvement of convergence, after its transformation to form [50]

$$\sigma_0 = -\eta C + \frac{1}{3}\eta^3 S - \frac{1}{5}\eta^5 D + \sum_{n=1}^{\infty}\left[\frac{\eta}{n} - \mathrm{arctg}\left(\frac{\eta}{n}\right) - \frac{1}{3}\frac{\eta^3}{n^3} + \frac{1}{5}\frac{\eta^5}{n^5}\right] , \tag{1.2.24}$$

where $D = \sum_{k=1}^{\infty} \frac{1}{k^5} = 1.036927751...$. Such series congregates very quickly and has the residual member of an order of η^7/n^6, so for the satisfaction of the accuracy stated above it is necessary to consider only a few tens of terms.

The program on the BASIC language for the calculation of the Coulomb phase shifts is given below, by the decomposition method described above in a row and on the basis of integrated representations (1.2.19) and series (1.2.24) – the description of some parameters is given in the program.

REM PROGRAM OF THE CALCULATION OF THE COULOMB PHASE SHIFTS

```
DEFDBL A-Z
DEFINT I,J,K,L,N,M
M=4000
DIM V(M): CLS
EPS=1.0E-15: REM CALCULATION ACCURACY
H=1: REM COULOMB PARAMETER
REM CALCULATION OF PHASE SHIFTS ON THE BASIS OF RANKS
C=0.577215665: A1=1.202056903/3: A2=1.036927755/5: F=0: S1=0
3 F=F+1
B=H/F-ATN(H/F)
S1=S1+B
IF B<EPS GOTO 2
GOTO 3
2 D=0: S=0
4 D=D+1
A=H/D-ATN(H/D)-(H/D)^3/3+(H/D)^5/5
S=S+A
IF A<EPS GOTO 1
GOTO 4
1 FAZ=-C*H+A1*H^3-A2*H^5+S
FAZ1=-C*H+S1
PRINT "FAZ = ";FAZ; "   N = ";D
PRINT "FAZ1 = ";FAZ1;"  N = ";F
```

```
REM *** CALCULATION OF THE PHASE SHIFTS ON THE BASIS OF INTEGRATED REPRESENTATION ***
NN=4000: E=1E-300: N=500: R1=0.1: R2=1: R3=40: HH=R1/N
H1=HH/NN: H2=(R2-R1)/NN: H3=(R3-R2)/NN: YY=0
FOR K=1 TO N
AA=(K-1)*HH
FOR I=0 TO NN
X=H1*I+AA+E
V(I)=EXP(-X)*SIN(H*LOG(X))
NEXT I
CALL SIM(NN,H1,V(),Y1)
YY=YY+Y1
NEXT K
FOR I=0 TO NN
X=H2*I+R1
V(I)=EXP(-X)*SIN(H*LOG(X))
NEXT
CALL SIM(NN,H2,V(),Y1)
YY=YY+Y1
FOR I=0 TO NN
X=H3*I+R2
V(I)=EXP(-X)*SIN(H*LOG(X))
NEXT
CALL SIM(NN,H3,V(),Y1)
YY=YY+Y1
XX=0
FOR K=1 TO N
AA=(K-1)*HH
FOR I=0 TO NN
X=H1*I+AA+E
V(I)=EXP(-X)*COS(H*LOG(X))
NEXT I
CALL SIM(NN,H1,V(),X1)
XX=XX+X1
NEXT K
FOR I=0 TO NN
```

```
X=H2*I+R1
V(I)=EXP(-X)*COS(H*LOG(X))
NEXT
CALL SIM(NN,H2,V(),X1)
XX=XX+X1
FOR I=0 TO NN
X=H3*I+R2
V(I)=EXP(-X)*COS(H*LOG(X))
NEXT
CALL SIM(NN,H3,V(),X1)
XX=XX+X1
AA=ATN(YY/XX)
PRINT "FAZA = ";AA
END

SUB SIM(N,H,V(5000),S)
A=0: B=0
FOR I=1 TO N-1 STEP 2
B=B+V(I)
NEXT
FOR J=2 TO N-2 STEP 2
A=A+V(J)
NEXT
S=H*(V(0)+V(N)+2*A+4*B)/3
END SUB
```

The phase shifts, given in tab. 1.2.1, are calculated according to this program on the basis of formula (1.2.24) [50]. The error makes about a half of the last sign.

Tab.1.2.1 - Calculation of the Coulomb phase shifts.

η	σ_0	η	σ_0
0.1	-0.05732294	0.6	-0.27274381
0.2	-0.11230222	0.8	-0.30422560
0.3	-0.16282067	1.0	-0.30164032

0.4	-0.20715583	1.3	-0.23921678
0.5	-0.24405830	1.5	-0.16293977

We will note that for the obtaining the identical accuracy at the calculating by formulae (1.2.24) and (1.2.22), in the last case, designated further as σ_1, it is necessary to consider approximately in seven hundred times more members of term (with an accuracy of 10^{-15}) that is clear from the given listing of results of the calculation at $\eta = 1$

$\sigma_0 = -0.30164032059$ for $N = 106$
$\sigma_1 = -0.30164032060$ for $N = 69337$

The calculation of the Coulomb phase shifts on the basis of integrated representation can be executed if to divide all intervals of integration into several parts. The most strongly subintegral function changes at small t, therefore we divide an integration interval into the following parts 0–0.1, 0.1–1 and 1–40 (at $t = 40$ subintegral function has a value 10^{-17} order), and the first part (0–0.1) we divide into $N = 500$ parts. The calculation of the integrals by all parts leads us to the phase shift value -0.30164031, that differs from the result obtained above on the basis of ranks only on unit of the eighth sign. We will note that the calculation of such integrals (1.2.19) on the Intel Pentium 200 MMX computer takes several minutes, and calculation of a row (1.2.24) – a fraction of a second.

1.2.7 Methods of the calculation of the Coulomb functions

Now we will pass to the consideration of the Coulomb scattering functions, regular $F_L(\eta,\rho)$ and irregular $G_L(\eta,\rho)$ parts of which are linearly independent solutions of the radial Schrödinger equation (1.2.1) only with a Coulomb potential, which has the form [6,9]

$$\chi_L''(\rho) + \left(1 - \frac{2\eta}{\rho} - \frac{L(L+1)}{\rho^2}\right)\chi_L(\rho) = 0 \ , \qquad (1.2.25)$$

where $\chi_L = F_L(\eta,\rho)$ or $G_L(\eta,\rho)$, $\rho = kr$, a $\eta = \frac{\mu Z_1 Z_2}{\hbar^2 k}$ – the Coulomb parameter. The Wronskian of these functions and their derivatives have the following appearance [6]

$$W_1 = F_L' G_L - F_L G_L' = 1,$$
$$W_2 = F_{L-1} G_L - F_L G_{L-1} = \frac{L}{\sqrt{\eta^2 + L^2}}. \qquad (1.2.26)$$

The recurrence relations are written in the form

$$L[(L+1)^2 + \eta^2]^{1/2} u_{L+1} = (2L+1)\left[\eta + \frac{L(L+1)}{\rho}\right] u_L - (L+1)[L^2 + \eta^2]^{1/2} u_{L-1},$$

$$(L+1) u_L' = \left[\frac{(L+1)^2}{\rho} + \eta\right] u_L - [(L+1)^2 + \eta^2]^{1/2} u_{L+1}, \qquad (1.2.27)$$

$$L u_L' = [L^2 + \eta^2]^{1/2} u_{L-1} - \left[\frac{L^2}{\rho} + \eta\right] u,$$

where $u_L = F_L(\eta,\rho)$ or $G_L(\eta,\rho)$. The asymptotics at $\rho \to \infty$ can be presented in the form [40]

$$F_L = \sin(\rho - \eta \ln 2\rho - \pi L/2 + \sigma_L),$$
$$G_L = \cos(\rho - \eta \ln 2\rho - \pi L/2 + \sigma_L). \qquad (1.2.28)$$

There are many methods and approximations for the calculation of the Coulomb functions [6,41,42,43,44,45,46,47]. However, the quickly converging representation allowing one to obtain their values with a fine precision and in the wide range of values of the variables with small expenses of the computer time [48] was appeared rather recently. The Coulomb functions in such method are presented in the form of continued fractions [49]

$$f_L = F_L^{'} / F_L = b_0 + \cfrac{a_1}{b_1 + \cfrac{a_2}{b_2 + \cfrac{a_3}{b_3 + ...}}}, \qquad (1.2.29)$$

where

$b_0 = (L + 1)/\rho + \eta/(L + 1)$,

$b_n = [2(L + n) + 1][(L + n)(L + n + 1) + \eta\rho]$,

$a_1 = - \rho[(L + 1)^2 + \eta^2](L + 2)/(L + 1)$,

$a_n = - \rho^2[(L + n)^2 + \eta^2][(L + n)^2 - 1]$

and

$$P_L + iQ_L = \frac{G_L^{'} + iF_L^{'}}{G_L + iF_L} = \frac{i}{\rho}\left(b_0 + \cfrac{a_1}{b_1 + \cfrac{a_2}{b_2 + \cfrac{a_3}{b_3 + ...}}} \right), \qquad (1.2.30)$$

where

$$b_0 = \rho - \eta, \qquad b_n = 2(b_0 + in),$$
$$a_n = - \eta^2 + n(n - 1) - L(L + 1) + i\eta(2n - 1). \qquad (1.2.31)$$

Such method of the calculation is applicable in the range at $\rho \geq \eta + \sqrt{\eta^2 + L(L+1)}$ and easily allows one to obtain the high precision thanks to the fast convergence of the continued fractions. As the Coulomb η parameter usually has the value unit order, and L, as a rule, no more than

3–5, the method yields the good results already at $\rho > 5$ fm. In this area it is necessary to know the Coulomb functions at numerical calculations of the nuclear functions of the scattering and reactions.

Using (1.2.29-1.2.31) it is possible to obtain the communication between the Coulomb functions and their derivatives [50,51]

$$F_L' = f_L F_L, \qquad (1.2.32)$$
$$G_L = (F_L' - P_L F_L)/Q_L = (f_L - P_L)F_L/Q_L,$$
$$G_L' = P_L G_L - Q_L F_L = [P_L(f_L - P_L)/Q_L - Q_L]F_L.$$

Thus, setting some F_L value in the ρ point, we find all other functions and their derivatives within the accuracy a constant multiplier, which is defined from Wronskian (1.2.26). The calculations of the Coulomb functions on the given formulae and comparison them with the tabular material [52] shows that it is possible to obtain easily eight-nine correct signs, if ρ meets the condition given above.

The text of the computer program for the calculation of the Coulomb scattering wave functions is given below. Here the following designations are accepted

G – Coulomb parameter,
L – orbital moment of this partial wave,
X – distance from the center, on which the Coulomb functions are calculated,
FF and GG – Coulomb functions,
FP and GP – their derivatives,
W – Wronskian, determining the accuracy of calculation of the Coulomb functions (The first formula in expression (1.2.26)).

```
SUB CULFUN(G,X,L,FF,GG,FP,GP,W)
REM SUBPROGRAMME OF CALCULATION OF THE COULOMB
FUNCTIONS *****
Q=G:R=X: GK=Q*Q: GR=Q*R:RK=R*R: K=1: F0=1
B01=(L+1)/R+Q/(L+1):BK=(2*L+3)*((L+1)*(L+2)+GR)
AK= - R*((L+1)^2+GK)/(L+1)*(L+2):DK=1/BK: DEHK=AK*DK
S=B01+DEHK
```

```
1 K=K+1
AK= - RK*((L+K)^2 - 1)*((L+K)^2+GK)
BK=(2*L+2*K+1)*((L+K)*(L+K+1)+GR)
DK=1/(DK*AK+BK)
IF DK>0 GOTO 3
2 F0= - F0
3 DEHK=(BK*DK - 1)*DEHK
S=S+DEHK
IF (ABS(DEHK) - 1E - 10)>0 GOTO 1
FL=S: K=1:RMG=R - Q
LL=L*(L+1): CK= - GK - LL:DK=Q: GKK=2*RMG
HK=2: AA1=GKK*GKK+HK*HK: PBK=GKK/AA1
RBK= - HK/AA1: OMEK=CK*PBK-DK*RBK
EPSK=CK*RBK+DK*PBK: PB=RMG+OMEK: QB=EPSK
4 K=K+1: CK= - GK - LL+K*(K - 1): DK=Q*(2*K - 1)
HK=2*K: FI=CK*PBK - DK*RBK+GKK: PSI=PBK*DK+RBK*CK+HK
AA2=FI*FI+PSI*PSI: PBK=FI/AA2: RBK= - PSI/AA2
VK=GKK*PBK - HK*RBK: WK=GKK*RBK+HK*PBK
OM=OMEK: EPK=EPSK
OMEK=VK*OM - WK*EPK - OM
EPSK=VK*EPK+WK*OM - EPK:
PB=PB+OMEK
QB=QB+EPSK
IF (ABS(OMEK)+ABS(EPSK) - 1E - 10)>0 GOTO 4
PL= - QB/R: QL=PB/R
G0=(FL - PL)*F0/QL
G0P=(PL*(FL - PL)/QL - QL)*F0
F0P=FL*F0
ALFA=1/(SQR(ABS(F0P*G0 - F0*G0P)))
GG=ALFA*G0
GP=ALFA*G0P
FF=ALFA*F0
FP=ALFA*F0P
W=1 - FP*GG+FF*GP
END SUB
```

The results of the control account of the Coulomb functions for $\eta = 1$ [53,54] and comparison them with the tabular data [52] are given in tab. 1.2.2. It is clear that at $\eta = 1$ and $L = 0$ the correct results turn out already for $\rho = kr = 1$. The value of the Wronskian (1.2.26) presented in the form $(W_1 - 1)$, at any ρ does not exceed 10^{-15}-10^{-16}.

Tab. 1.2.2 - Coulomb functions.

ρ	F_0 (Our calculation)	F_0 *[52]*	F_0' (Our calculation)	F_0' *[52]*
1	0.22752621	0.22753	0.34873442	0.34873
5	0.68493741	0.68494	-0.72364239	-0.72364
10	0.47756082	0.47756	0.84114311	0.84114
15	-0.97878958	-0.97879	0.31950815	0.31951
20	-0.32922554	-0.32923	-0.92214689	-0.92215
ρ	G_0	G_0 *[52]*	G_0'	G_0' *[52]*
1	2.0430972	2.0431	-1.2635981	-1.2636
5	-0.89841436	-0.89841	-0.51080476	-0.51080
10	0.94287424	0.94287	-0.43325965	-0.43326
15	0.34046374	0.34046	0.91053182	0.91053
20	-0.97242840	-0.97243	0.31370038	0.31370
ρ	F_2	G_2	F'_2	G'_2
1	1.47867E-02	1.26407E 01	4.70896E-02	-2.73727E 01
5	1.18637E 00	3.82961E-01	1.54145E-01	-7.93149E-01
10	-9.63615E-01	4.81305E-01	4.24848E-01	8.25557E-01
15	-2.27973E-01	-1.01918E 00	-9.33599E-01	2.12743E-01
20	-1.01801E 00	-1.62845E-01	-1.55072E-01	-9.57506E-01

The correctness of the function's calculation at $L = 2$ is easy to check on the recurrent formulae (1.2.27). Knowing the functions and their derivatives at $L = 0$, on the second formula (1.2.27) we find the functions at $L = 1$, and then, on the third formula, we find their derivatives for $L = 1$. Continuing this process is easy to find all functions and their derivatives at any L [50].

Now we will provide the text of the same computer program for calculation of the Coulomb scattering wave functions in the algorithmic language Fortran-90. The designation of the parameters practically coincides with the previous program. Here on the basis of (1.2.29) and (1.2.30) only functions are defined at $L = 0$, and for the finding of functions at all other L the recurrence relations are used. For ensuring the greatest possible accuracy of the results, as well as in the previous case, the mode of the double accuracy is used. Here the following designations are accepted

Q – Coulomb parameter η,
LM – orbital moment of this partial wave,
R – distance from the center, on which the Coulomb functions are calculated,
F and G – Coulomb functions,
W – Wronskian, determining the accuracy of the calculation of the Coulomb functions (The first formula in expression (1.2.26)).

```
SUBROUTINE CULFUN(LM,R,Q,F,G,W)
! SUBPROGRAMME OF CALCULATION OF THE COULOMB
! FUNCTIONS
IMPLICIT REAL(8) (A-Z)
INTEGER L,K,LL,LM
EP=1.0D-015; L=0; F0=1.0D-000
GK=Q*Q; GR=Q*R; RK=R*R
B01=(L+1)/R+Q/(L+1)
K=1; BK=(2*L+3)*((L+1)*(L+2)+GR)
AK=-R*((L+1)**2+GK)/(L+1)*(L+2)
DK=1.0D-000/BK
DEHK=AK*DK
S=B01+DEHK
15 K=K+1
AK=-RK*((L+K)**2-1)*((L+K)**2+GK)
BK=(2*L+2*K+1)*((L+K)*(L+K+1)+GR)
DK=1.D-000/(DK*AK+BK)
IF (DK>0.0D-000) GOTO 35
25 F0=-F0
```

```
35 DEHK=(BK*DK-1.0D-000)*DEHK
S=S+DEHK
IF (ABS(DEHK)>EP) GOTO 15
FL=S; K=1; RMG=R-Q; LL=L*(L+1)
CK=-GK-LL; DK=Q; GKK=2.0D-000*RMG
HK=2.0D-000; AA1=GKK*GKK+HK*HK
PBK=GKK/AA1; RBK=-HK/AA1
AOMEK=CK*PBK-DK*RBK
EPSK=CK*RBK+DK*PBK
PB=RMG+AOMEK; QB=EPSK
52 K=K+1
CK=-GK-LL+K*(K-1); DK=Q*(2*K-1)
HK=2.0D-000*K; FI=CK*PBK-DK*RBK+GKK
PSI=PBK*DK+RBK*CK+HK
AA2=FI*FI+PSI*PSI; PBK=FI/AA2
RBK=-PSI/AA2; VK=GKK*PBK-HK*RBK
WK=GKK*RBK+HK*PBK; OM=AOMEK
EPK=EPSK; AOMEK=VK*OM-WK*EPK-OM
EPSK=VK*EPK+WK*OM-EPK; PB=PB+AOMEK
QB=QB+EPSK
IF ((ABS(AOMEK)+ABS(EPSK))>EP) GOTO 52
PL=-QB/R; QL=PB/R
G0=(FL-PL)*F0/QL; G0P=(PL*(FL-PL)/QL-QL)*F0; F0P=FL*F0
ALFA=1.0D-000/DSQRT(ABS(F0P*G0-F0*G0P))
G=ALFA*G0; GP=ALFA*G0P
F=ALFA*F0; FP=ALFA*F0P
W=1.0D-000-FP*G+F*GP
IF (LM==0) GOTO 123
AA=DSQRT(1.0D-000+Q**2)
BB=1.0D-000/R+Q
F1=(BB*F-FP)/AA
G1=(BB*G-GP)/AA
WW1=F*G1-F1*G-1.0D-000/DSQRT(Q**2+1.0D-000)
IF (LM==1) GOTO 234
DO L=1,LM-1
AA=DSQRT((L+1)**2+Q**2)
```

```
BB=(L+1)**2/R+Q
CC=(2*L+1)*(Q+L*(L+1)/R)
DD=(L+1)*DSQRT(L**2+Q**2)
F2=(CC*F1-DD*F)/L/AA
G2=(CC*G1-DD*G)/L/AA
WW2=F1*G2-F2*G1-(L+1)/DSQRT(Q**2+(L+1)**2)
F=F1; G=G1; F1=F2; G1=G2
ENDDO
234 F=F1; G=G1
123 END
```

This program yields just the same results of the control account as previous in the Turbo Basic language.

1.3 Program of the calculation of phase shifts for the central real potentials

Now we will provide the computer program for calculation of the real phase shifts of the elastic scattering by the finite-difference method and the Runge-Kutt method in the Basic language, which shows a good coincidence of the results obtained by the both ways. Here the following designations are accepted:

NN – Lower value of the energy cycle,
NV – Top value of the energy cycle,
NH – Step by the energy cycle,
EH – Step by the energy,
EN – The lower value by the energy,
AM1 – The mass of the first particle in amu,
AM2 – The mass of the second particle in amu,
PM – The reduced mass of μ,
Z1 – A charge of the first particle in terms of a charge "e",
Z2 – A charge of the second particle in terms of a charge "e",
A1 – $\hbar^2/M_N = 41.4686$ constant, where M_N - the mass of a nucleon in amu, equal 1,
AK1 – constant at Coulomb potential $1.439975\ Z_1Z_2\ 2\mu/\hbar^2$,
N – Number of steps at the integration of the Schrödinger equation,
H – Step value at the integration of the Schrödinger equation,
R00 – Distance, at which the lacing of the numerical functions with an asymptotics is carried out,
V0 – Depth of the nuclear potential,
R0 – Radius of the nuclear potential,
RCU – Coulomb radius,
L – Orbital moment,
EL – Energy of particles in the laboratory system,
ECM – Energy of particles in system of the center of masses,
SK – Square of the k^2 wave number,
SS – Wave number k,
G – Coulomb parameter = $3.44476\ 10^{-2}\ Z_1Z_2\ \mu/k$,
F1(I) – The phase shift shifts at the set energy obtained by the finite-

difference method,

F2(I) – The phase shift shifts at the set energy obtained by the Runge-Kutt method,

ABS(F1(I) - F2(I)) – A difference of phase shifts in the degrees obtained by the different methods

ABS(F1(I) - F2(I))/ABS(F1(I))*100 – a relative difference of the phase shifts in percentage.

REM PROGRAM OF CALCULATION OF THE REAL PHASE SHIFT SHIFTS

```
 REM *** DETERMITION OF MASSIFS AND VARIABLES ****
 DEFDBL A - Z: DEFINT I,J,K,L,N,M: CLS
 NN=4000: DIM EL(100), F1(100), ECM(100), F2(100)
 DIM V1(NN), U(NN), V(NN), U1(NN)
 PRINT "  EL  ECM  FKR  FRK  ERR - DEG  ERR - %"
REM ***** DETERMINATION OF THE INITIAL VALUES ******
 PI=3.14159265359: NN=1: NV=20: NH=1: EH=1: EN=0
 AM1=2: AM2=4: Z1=1: Z2=2: A1=41.4686
  PM=AM1*AM2/(AM1+AM2)
 B1=2*PM/A1: AK1=1.439975*Z1*Z2*B1: N=1000: R00=20: H=R00/N
 V0=76.12: R0=.2: A2= - V0*B1: RCU=0: L=0
REM *********** BEGINNING OF THE CYCLE ON ENERGY ******
 FOR  I=NN  TO  NV  STEP  NH:  EL(I)=EN+EH*I:
ECM(I)=EL(I)*PM/AM1
 SK=ECM(I)*B1: SS=SQR(SK): G=3.44476E - 02*Z1*Z2*PM/SS
REM ***** CALCULATION OF THE COULOMB FUNCTIONS *****
 X1=H*SS*(N - 4): X2=H*SS*(N): CALL CUL(G,X1,L0,F1,G1,W1)
 CALL CUL(G,X2,L0,F2,G2,W2)
REM *** CALCULATION OF THE PHASE SHIFTS OF BY THE
FINITE-DIFFERENCE METHOD ***
 CALL FUN(N,H,U1(),L,A2,AK1,SK,R0,RCU)
 D1=U1(N - 4): D2=U1(N): AF= - (F1 - F2*D1/D2)/(G1 - G2*D1/D2)
 FF=ATN(AF): IF FF>0 GOTO 90: FF=FF+PI
90 XN1=(COS(FF)*F2+SIN(FF)*G2)/D2: F1(I)=FF*180/PI
REM *** CALCULATION OF THE PHASE SHIFTS BY THE RUNGE-
KUTT METHOD***
```

```
 CALL FUNRK(V(),N,H): D1=V(N - 4): D2=V(N)
 AF= - (F1 - F2*D1/D2)/(G1 - G2*D1/D2): F33=ATN(AF)
 IF F33>0 GOTO 91: F33=F33+PI
91 XN2=(COS(F33)*F2+SIN(F33)*G2)/D2: F2(I)=F33*180/PI
REM ********* PHASE SHIFT PRINTING ***************
 PRINT USING "+#.####^^^^ "; EL(I); ECM(I); F1(I); F2(I); ABS(F1(I) -
F2(I)); ABS(F1(I) - F2(I))/ABS(F1(I))*100: NEXT I
STOP

 SUB CUL(G,X,L,F0,G0,W)
REM CALCULATION OF COULOMB SCATTERING FUNCTIONS
 Q=G: R=X: F0=1: K=1: GK=Q*Q: GR=Q*R: RK=R*R
 B01=(L+1)/R+Q/(L+1): BK=(2*L+3)*((L+1)*(L+2)+GR)
 AK= - R*((L+1)^2+GK)/(L+1)*(L+2): DK=1/BK: DEHK=AK*DK
 S=B01+DEHK
1 K=K+1: AK= - RK*((L+K)^2 - 1)*((L+K)^2+GK)
 BK=(2*L+2*K+1)*((L+K)*(L+K+1)+GR): DK=1/(DK*AK+BK)
 IF DK>0 GOTO 3
2 F0= - F0
3 DEHK=(BK*DK - 1)*DEHK: S=S+DEHK
 IF (ABS(DEHK) - 1E - 06)>0 GOTO 1: FL=S: K=1: RMG=R - Q
 LL=L*(L+1): CK= - GK - LL: DK=Q: GKK=2*RMG: HK=2
 AA1=GKK*GKK+HK*HK: PBK=GKK/AA1: RBK= - HK/AA1
 OMEK=CK*PBK - DK*RBK: EPSK=CK*RBK+DK*PBK
 PB=RMG+OMEK: QB=EPSK
5 K=K+1: CK= - GK - LL+K*(K - 1): DK=Q*(2*K - 1): HK=2*K
 FI=CK*PBK - DK*RBK+GKK: PSI=PBK*DK+RBK*CK+HK
 AA2=FI*FI+PSI*PSI: PBK=FI/AA2: RBK= - PSI/AA2
 VK=GKK*PBK - HK*RBK: WK=GKK*RBK+HK*PBK
 OM=OMEK: EPK=EPSK: OMEK=VK*OM - WK*EPK - OM
 EPSK=VK*EPK+WK*OM - EPK: PB=PB+OMEK: QB=QB+EPSK
 IF (ABS(OMEK)+ABS(EPSK) - 1E - 06)>0 GOTO 5: PL= - QB/R
 QL=PB/R: G0=(FL - PL)*F0/QL: G0P=(PL*(FL - PL)/QL - QL)*F0
 F0P=FL*F0: ALFA=1/(SQR(ABS(F0P*G0 - F0*G0P))): G0=ALFA*G0
 GP=ALFA*G0P: F0=ALFA*F0: FP=ALFA*F0P: W=1 - FP*G0+F0*GP
 END SUB
```

```
SUB FUN(N,H,U(5000),L,AV,AK,SK,R0,RCU)
REM ***** THE SOLUTION OF THE SCHRÖDINGER EQUATION
BY THE FINITE-DIFFERENCE METHOD *****
U(0)=0: U(1)=0.001: HK=H*H: FOR K=1 TO N - 1: X=K*H
Q1=AV*EXP( - R0*X*X)+L*(L+1)/(X*X): IF X>RCU GOTO 11
Q1=Q1+(3 - (X/RCU)^2)*AK/(2*RCU): GOTO 22
11 Q1=Q1+AK/X
22 Q2= - Q1*HK - 2+SK*HK: U(K+1)= - Q2*U(K) - U(K - 1): NEXT K
END SUB

SUB FUNRK(V(5000),N,H)
REM ****** THE SOLUTION OF THE SCHRÖDINGER EQUATION
BY THE RUNGE-KUTT METHOD IN ALL AREA OF VARIABLES **
VA1=0: REM VA1 – The value of the function in zero
PA1=1.0E - 05: REM PA1 - The value of function on the first step
FOR I=0 TO N - 1: X=H*I+1.0E - 05
CALL RRUN(VB1,PB1,VA1,PA1,H,X)
VA1=VB1: PA1=PB1: V(I+1)=VA1: NEXT
END SUB

SUB RRUN(VB1,PB1,VA1,PA1,H,X)
REM ***** THE SOLUTION OF THE SCHRÖDINGER EQUATION
BY THE RUNGE-KUTT METHOD BY THE ONE STEP *****
X0=X: Y1=VA1: CALL F(X0,Y1,FK1): FK1=FK1*H: FM1=H*PA1
X0=X+H/2: Y2=VA1+FM1/2: CALL F(X0,Y2,FK2): FK2=FK2*H
FM2=H*(PA1+FK1/2): Y3=VA1+FM2/2: CALL F(X0,Y3,FK3)
FK3=FK3*H: FM3=H*(PA1+FK2/2): X0=X+H: Y4=VA1+FM3
CALL F(X0,Y4,FK4): FK4=FK4*H: FM4=H*(PA1+FK3)
PB1=PA1+(FK1+2*FK2+2*FK3+FK4)/6
VB1=VA1+(FM1+2*FM2+2*FM3+FM4)/6: END SUB

SUB F(X,Y,F)
REM * FUNCTION EVALUATION OF F (X, Y) IN THE RUNGE-KUTT
METHOD *
SHARED SK,A2,R0,AK1,L,RCU
VC=A2*EXP(-R0*X^2): IF X>RCU GOTO 121
```

```
VK=(3-(X/RCU)^2)*AK1/(2*RCU): GOTO 222
121 VK=AK1/X
222 F=-(SK-VK-VC-L*(L+1)/(X^2))*Y
END SUB
```

For carrying out of the control account we used a finite-difference method with the classical nucleon-nucleon Reid potential [55]. The form of ${}^1P_1$ potential and calculation scattering phase shifts are given in this work. Our calculations of phase shifts with such potential are given in tab. 1.3.1 in the comparison with the Reid results.

Tab. 1.3.1 - Comparison of the results for the Reid potential.

E, MeV	δ, radian, [55]	δ, radian, (Our calculation)
48	-0.071	-0.072
144	-0.312	-0.314
208	-0.456	-0.458
352	-0.708	-0.710

It is clear from these results that the coincidence of both calculations with the accuracy about several thousand of radian, that is a fine example of the efficiency of the used numerical methods and the accuracy of work of the described program.

Now we will compare the accuracy, with which it is possible to obtain the phase shift shifts by two considered methods – the Runge-Kutt and finite-difference. We will give the results of calculations of phase shifts by two of these methods (FDM – finite-difference and RKM – Runge-Kutt) for the S scattering phase shift in the ${}^2H{}^4He$ system (parameters of the potential are obtained by us in works [56] $V_0 = 76.12$ MeV, $\alpha = 0.2$ fm^{-2}, $R_c = 0$ fm, $L = 0$ and represent the alternative variant of the similar potentials for the first time offered in works [57,58,59,60]) and extent of their coincidence in degrees (ERR - DEG) and percent (ERR - %) [61]. Here EL, ECM - the energy in the laboratory system and system of the center of mass of the colliding particles.

EL	ECM	FKR	FRK	ERR - DEG	ERR - %
+1.0000E+00	+6.6667E-01	+1.5053E+02	+1.5052E+02	+8.4828E-03	+5.6353E-03
+2.0000E+00	+1.3333E+00	+1.2598E+02	+1.2597E+02	+1.2241E-02	+9.7170E-03
+3.0000E+00	+2.0000E+00	+1.0892E+02	+1.0890E+02	+1.4219E-02	+1.3055E-02
+4.0000E+00	+2.6667E+00	+9.5886E+01	+9.5871E+01	+1.5547E-02	+1.6214E-02
+5.0000E+00	+3.3333E+00	+8.5335E+01	+8.5319E+01	+1.6536E-02	+1.9378E-02
+6.0000E+00	+4.0000E+00	+7.6457E+01	+7.6440E+01	+1.7629E-02	+2.3057E-02
+7.0000E+00	+4.6667E+00	+6.8801E+01	+6.8782E+01	+1.8828E-02	+2.7365E-02
+8.0000E+00	+5.3333E+00	+6.2083E+01	+6.2063E+01	+1.9867E-02	+3.2000E-02
+9.0000E+00	+6.0000E+00	+5.6102E+01	+5.6081E+01	+2.0743E-02	+3.6974E-02
+1.0000E+01	+6.6667E+00	+5.0715E+01	+5.0693E+01	+2.1731E-02	+4.2848E-02
+1.1000E+01	+7.3333E+00	+4.5818E+01	+4.5795E+01	+2.2996E-02	+5.0189E-02
+1.2000E+01	+8.0000E+00	+4.1334E+01	+4.1310E+01	+2.4399E-02	+5.9028E-02
+1.3000E+01	+8.6667E+00	+3.7206E+01	+3.7180E+01	+2.5677E-02	+6.9014E-02
+1.4000E+01	+9.3333E+00	+3.3383E+01	+3.3356E+01	+2.6730E-02	+8.0071E-02
+1.5000E+01	+1.0000E+01	+2.9825E+01	+2.9798E+01	+2.7712E-02	+9.2913E-02
+1.6000E+01	+1.0667E+01	+2.6500E+01	+2.6471E+01	+2.8870E-02	+1.0894E-01
+1.7000E+01	+1.1333E+01	+2.3379E+01	+2.3349E+01	+3.0323E-02	+1.2970E-01

The worse result is shown in the last line and makes 0.13% at energy of 17 MeV. Furthermore, we will give the results of calculations of the $S_{1/2}$ phase shift for the elastic $^3H^4He$ scattering at low energies by [61] two methods. For parameters of the potential the following values – V_0 = -67.5 MeV, α = 0.15747 fm^{-2}, R_c = 3.095 fm, L = 0 [56,61] are used.

EL	ECM	FKR	FRK	ERR - DEG	ERR - %
+1.0000E-01	+4.2857E-02	+1.8000E+02	+1.8000E+02	+3.0506E-07	+1.6948E-07
+1.1000E+00	+4.7143E-01	+1.7204E+02	+1.7204E+02	+1.2686E-03	+7.3739E-04
+2.1000E+00	+9.0000E-01	+1.6139E+02	+1.6138E+02	+2.8364E-03	+1.7575E-03
+3.1000E+00	+1.3286E+00	+1.5211E+02	+1.5211E+02	+4.0288E-03	+2.6486E-03
+4.1000E+00	+1.7571E+00	+1.4419E+02	+1.4419E+02	+4.9487E-03	+3.4320E-03
+5.1000E+00	+2.1857E+00	+1.3729E+02	+1.3729E+02	+5.6562E-03	+4.1198E-03
+6.1000E+00	+2.6143E+00	+1.3113E+02	+1.3113E+02	+6.2638E-03	+4.7767E-03
+7.1000E+00	+3.0429E+00	+1.2555E+02	+1.2555E+02	+6.8101E-03	+5.4240E-03
+8.1000E+00	+3.4714E+00	+1.2045E+02	+1.2044E+02	+7.2653E-03	+6.0317E-03
+9.1000E+00	+3.9000E+00	+1.1574E+02	+1.1573E+02	+7.6262E-03	+6.5892E-03
+1.0100E+01	+4.3286E+00	+1.1134E+02	+1.1133E+02	+7.9425E-03	+7.1336E-03
+1.1100E+01	+4.7571E+00	+1.0721E+02	+1.0720E+02	+8.2671E-03	+7.7111E-03
+1.2100E+01	+5.1857E+00	+1.0331E+02	+1.0330E+02	+8.6088E-03	+8.3328E-03
+1.3100E+01	+5.6143E+00	+9.9620E+01	+9.9611E+01	+8.9358E-03	+8.9699E-03
+1.4100E+01	+6.0429E+00	+9.6112E+01	+9.6103E+01	+9.2141E-03	+9.5868E-03

+1.5100E+01 +6.4714E+00 +9.2768E+01 +9.2759E+01 +9.4404E-03 +1.0176E-02
+1.6100E+01 +6.9000E+00 +8.9572E+01 +8.9563E+01 +9.6453E-03 +1.0768E-02
+1.7100E+01 +7.3286E+00 +8.6509E+01 +8.6499E+01 +9.8700E-03 +1.1409E-02
+1.8100E+01 +7.7571E+00 +8.3566E+01 +8.3556E+01 +1.0139E-02 +1.2133E-02

The deviation of these results for the last line does not exceed 0.012%.

All these results show that the accuracy of the phase shifts of nuclear scattering obtained from these calculations by both methods is at the level of tenth-hundredth shares of percent and any of these ways can be applied to the real calculations of nuclear phase shifts of the elastic scattering in any cluster systems with the central forces.

Now we will provide the text of the computer program for the calculations of the elastic scattering phase shifts, in this case, of protons on ^{7}Li, in the Fortran-90 language. The program carries out the calculation of the elastic scattering phase shifts of two particles for scattering wave function, by the methods, which are in detail described above with a given accuracy of the result. In this case, the absolute accuracy makes 10^{-3} radians. Passing to the computer program, we will notice that the description of the parameters of calculation, variables, the interaction potential, blocks of the program and subprogrammes is given in listing of the program.

PROGRAM FAZ_p7Li

```
! THE PROGRAM OF CALCULATION OF PHASE SHIFTS OF SCATTERING FOR THE SET ACCURACY
IMPLICIT REAL(8) (A-Z)
INTEGER(4) I,L,N
REAL(8) FA1(0:1000),ECM(0:1000),EL(0:1000)
DIMENSION U1(0:1024000)
! ***************** The nuclear data ********************
AM1=1.00727646577D-000; ! The P mass
AM2=7.01600455D-000 ! The 7Li mass
Z1=1.0D-000 ! The P charge
Z2=3.0D-000        ! The 7Li charge
PI=4.0D-000*DATAN(1.0D-000) ! The Pi number
PM=AM1*AM2/(AM1+AM2) ! The reduced mass
```

```
! ***************** The constants ************************
A1=41.4686D+00
B1=2.0D-000*PM/A1
AK1=1.439975D+00*Z1*Z2*B1
GK=3.44476D-02*Z1*Z2*PM
! ***************** The initial values ****************
NN=0 ! The initial value of a step
NV=30 ! The number of steps at calculation of the phase shifts
NH=1 ! The step value
EH=0.01D-000 ! The step in MeV for the calculation of the phase shifts
EN=0.3D-000  ! The lower value of energy of the calculation of the phase
shifts
EPF=1.0D-003 ! The accuracy of the calculation of the phase shifts
! *************** The potentials ************************
V0=1685.783D-000 ! The potential depth in MeV of the attracting part
R0=1.D-000 ! The potential radius of the attracting part in Fm
V1=0.0D-000 ! The potential depth in MeV of the repellent part
R1=1.0D-000 ! The potential radius of the repellent part in Fm
A0=-V0*B1; A1=V1*B1 ! The recalculation of depth of potentials in Fm^-2
RCU=0.0D-000 ! The coulomb radius in Fm
L=1 ! The orbital moment
! ************ The parameters for finding of the phase shifts ********
DO I=NN,NV,NH
N=1000 ! The initial number of steps of calculation of the WF
RR=10.0D-000 ! The initial distance for calculation of the WF
H=RR/N ! The initial distance for calculation of the WF
EL(I)=EN+I*EH ! The energy in a lab. system
ECM(I)=EL(I)*PM/AM1 ! The recalculation of energy in system of the
center of masses
SK=ECM(I)*B1 ! The square of the number
SS1=DSQRT(SK) ! The wave number
G=GK/SS1 ! Coulomb parameter
! ******* The subprogramme of calculation of the phase shift shifts *****
CALL
FAZ(G,SS1,I,RR,EPF,N,PI,H,L,U1,FA1,A0,A1,R0,R1,RCU,AK1,SK)
PRINT *,EL(I)*1000,FA1(I)
```

```
ENDDO
! ******************** The record of results in the file *********
OPEN (1,FILE='FAZ-P-7Li.DAT')
DO I=NN,NV,NH
WRITE(1,*) EL(I)*1000,FA1(I)
ENDDO
CLOSE(1)
END

SUBROUTINE FUN(N,H,A0,A1,R0,R1,L,RCU,AK,SK,U)
! *** The subprogramme of calculation of the wave function ***********
IMPLICIT REAL(8) (A-Z)
INTEGER(4) K,L,N
DIMENSION U(0:1024000)
U(0)=0.0D-000
U(1)=0.010D-000
HK=H*H
DO K=1,N-1
X=K*H
Q1=A0*DEXP(-R0*X*X)+L*(L+1)/(X*X)+A1*DEXP(-R1*X*X)
IF (X>RCU) GOTO 1157
Q1=Q1+(3.0D-000-(X/RCU)**2)*AK/(2.0D-000*RCU)
GOTO 1158
1157 Q1=Q1+AK/X
1158 Q2=-Q1*HK-2.0D-000+SK*HK
U(K+1)=-Q2*U(K)-U(K-1)
ENDDO
END

SUBROUTINE FAZ(G,SS,I,RR,EPF,N,PI,H,L,U,FA,A0,A1,
R0,R1,RCU,AK,SK)
! ************ The subprogramme of calculation of the phase shifts ****
IMPLICIT REAL(8) (A-Z)
INTEGER(4) N,L,I
DIMENSION U(0:1024000),FA(0:1000)
FN=1000.0; FR=1000.0
```

```
125 X1=H*SS*(N-4)
X2=H*SS*N
CALL CULFUN(L,X1,G,F1,G1,W0,EP)
CALL CULFUN(L,X2,G,F2,G2,W0,EP)
CALL FUN(N,H,A0,A1,R0,R1,L,RCU,AK,SK,U)
U10=U(N-4); U20=U(N)
AF=-(F1-F2*U10/U20)/(G1-G2*U10/U20)
F=DATAN(AF)
IF(F<0.0D-000) THEN
F=F+PI
ENDIF
IF(ABS(F)<1.0D-10) THEN
F=0.0D-000
ENDIF
IF (ABS(FN-F)>EPF) THEN
FN=F
N=N+100
H=RR/N
GOTO 125
ENDIF
IF (ABS(FR-F)>EPF) THEN
FR=F
RR=RR+1
N=N+0.2*N
H=RR/N
GOTO 125
ENDIF
FA(I)=F*180.0D-000/PI
END

SUBROUTINE CULFUN(LM,R,Q,F,G,W,EP)
! **** Subprogramme of the calculation of the Coulomb functions *****
IMPLICIT REAL(8) (A-Z)
INTEGER L,K,LL,LM
EP=1.0D-015
L=0
```

```
F0=1.0D-000
GK=Q*Q
GR=Q*R
RK=R*R
B01=(L+1)/R+Q/(L+1)
K=1
BK=(2*L+3)*((L+1)*(L+2)+GR)
AK=-R*((L+1)**2+GK)/(L+1)*(L+2)
DK=1.0D-000/BK
DEHK=AK*DK
S=B01+DEHK
15 K=K+1
AK=-RK*((L+K)**2-1.D-000)*((L+K)**2+GK)
BK=(2*L+2*K+1)*((L+K)*(L+K+1)+GR)
DK=1.D-000/(DK*AK+BK)
IF (DK>0.0D-000) GOTO 35
25 F0=-F0
35 DEHK=(BK*DK-1.0D-000)*DEHK
S=S+DEHK
IF (ABS(DEHK)>EP) GOTO 15
FL=S
K=1
RMG=R-Q
LL=L*(L+1)
CK=-GK-LL
DK=Q
GKK=2.0D-000*RMG
HK=2.0D-000
AA1=GKK*GKK+HK*HK
PBK=GKK/AA1
RBK=-HK/AA1
AOMEK=CK*PBK-DK*RBK
EPSK=CK*RBK+DK*PBK
PB=RMG+AOMEK
QB=EPSK
52 K=K+1
```

```
CK=-GK-LL+K*(K-1.)
DK=Q*(2.*K-1.)
HK=2.*K
FI=CK*PBK-DK*RBK+GKK
PSI=PBK*DK+RBK*CK+HK
AA2=FI*FI+PSI*PSI
PBK=FI/AA2
RBK=-PSI/AA2
VK=GKK*PBK-HK*RBK
WK=GKK*RBK+HK*PBK
OM=AOMEK
EPK=EPSK
AOMEK=VK*OM-WK*EPK-OM
EPSK=VK*EPK+WK*OM-EPK
PB=PB+AOMEK
QB=QB+EPSK
IF (( ABS(AOMEK)+ABS(EPSK) )>EP) GOTO 52
PL=-QB/R
QL=PB/R
G0=(FL-PL)*F0/QL
G0P=(PL*(FL-PL)/QL-QL)*F0
F0P=FL*F0
ALFA=1.0D-000/( (ABS(F0P*G0-F0*G0P))**0.5 )
G=ALFA*G0
GP=ALFA*G0P
F=ALFA*F0
FP=ALFA*F0P
W=1.0D-000-FP*G+F*GP
IF (LM==0) GOTO 123
AA=(1.0D-000+Q**2)**0.5
BB=1.0D-000/R+Q
F1=(BB*F-FP)/AA
G1=(BB*G-GP)/AA
WW1=F*G1-F1*G-1.0D-000/(Q**2+1.0D-000)**0.5
IF (LM==1) GOTO 234
DO L=1,LM-1
```

```
AA=((L+1)**2+Q**2)**0.5
BB=(L+1)**2/R+Q
CC=(2*L+1)*(Q+L*(L+1)/R)
DD=(L+1)*(L**2+Q**2)**0.5
F2=(CC*F1-DD*F)/L/AA
G2=(CC*G1-DD*G)/L/AA
WW2=F1*G2-F2*G1-(L+1)/(Q**2+(L+1)**2)**0.5
F=F1; G=G1; F1=F2; G1=G2
ENDDO
234 F=F1; G=G1
123 CONTINUE
END
```

Now we will give the results of the control account on this program for the elastic scattering of protons on ^{7}Li in P wave, i.e. at $L = 1$, with a potential specified in the program. Here E – energy of particles in keV, δ – a phase shift in degrees. Inscriptions for these values (E and δ) are not provided in the program.

E, keV	δ, degree
300.000000000000000	1.463012825309583
310.000000000000000	1.741580427189647
320.000000000000000	2.045211169193295
329.999999999999900	2.453917192921778
339.999999999999900	2.942034339443802
350.000000000000000	3.523983257335034
360.000000000000000	4.304066622497790
370.000000000000000	5.290031443719053
380.000000000000000	6.616684565601776
390.000000000000000	8.497854783693313
400.000000000000000	11.283887289718910
410.000000000000000	15.871292305763380
420.000000000000000	24.460811168704080
430.000000000000000	44.290494570708410
440.000000000000000	90.056769406018120
449.999999999999900	131.858294233151700

459.999999999999900	149.289857654389200
470.000000000000000	157.183982976260500
480.000000000000000	161.471562673128100
490.000000000000000	164.171993502029300
500.000000000000000	165.996407865298600
510.000000000000000	167.276268596475400
520.000000000000000	168.211429040413200
530.000000000000000	168.940799322204100
540.000000000000000	169.548066545885000
550.000000000000000	170.004755252677600
560.000000000000000	170.371698377092600
570.000000000000100	170.660104736125200
580.000000000000100	170.910851757862900
590.000000000000000	171.148334224319700
600.000000000000000	171.325330286482400

It is clear from these results that at 440 keV the P_1 phase shift reaches the resonance value in 90°, which really is at energy of 441 keV [28].

1.4 Program of calculation of the scattering phase shifts for the central complex potentials

Now we will provide the program for the calculation of complex phase shifts of the elastic scattering by the finite-difference method in the Basic language. Here the following designations are accepted

NN – The lower value of a cycle by the energy,
NV – The top value of a cycle by the energy,
LN – The lower value of the orbital moment,
LV – The top value of the orbital moment,
LH – A step on the values of the orbital moment,
AM1 – The mass of the first particle in amu,
AM2 – The mass of the second particle in amu,
PM – The reduced mass of μ,
Z1 – A charge of the first particle in terms of a charge "e",
Z2 – A charge of the second particle in terms of a charge "e",
A1 – A constant $\hbar^2/M_N = 41.4686$, where M_N - the mass of a nucleon in amu, equal to 1,
AK – A constant at the Coulomb potential $1.439975\ Z_1Z_2\ 2\mu/\hbar^2$,
N – Number of steps at the integration of the Schrödinger equation,
HH – A step value at integration of the Schrödinger equation,
R00 – A distance, at which the lacing of numerical functions with an asymptotics is carried out,
VR1 – The depth of the real potential,
RRR – The radius of the real potential,
AR - The diffusivity of the real potential of the Woods-Saxon potential,
VC1 - The depth of the imaginary part of potential,
RRC – The radius of the imaginary part of potential,
AC – The diffusivity of the imaginary part of the Woods-Saxon potential,
RCU – The coulomb radius,
L – The orbital moment,
E1 () – The energy of particles in the laboratory system,
E () – The energy of particles in the system of the center of masses,
SK – The square of the wave number of k^2,
SS – The k wave number,

GG – The coulomb parameter = 3.44476 10^{-2} Z_1Z_2 μ/k.

REM ** THE CALCULATION OF THE COMPLEX SCATTERING PHASE SHIFTS

```
 CLS: DEFDBL A-Z: DEFINT I,J,K,L,N,M: NN=4000: N=100
 DIM E(N), DE(N), DEE(N), FAZA(N,15), E1(N), X(NN), Y(NN),
ETA(N,15), SIG(N,15), SEC(N), FAZ(N,15)
 DIM V(NN),W(NN),FM(20),FR(20),FR1(20),FM1(20),ET(N)
 REM  ****************************************
A$ =" THE COMPLEX PHASE SHIFTS"
 B$="   E(CM)        FAZR(EXP)     FAZR(TEOR)    FAZC(EXP)
FAZC(TEOR)  ETA(TEOR) "
 SAVE=0: G$="C:\BASICA\FAZCOM\FAZALAL1.DAT"
 PRINT "-----------------------------------------------------------": PRINT
B$
REM ************ THE TYPE OF THE POTENTIALS ************
 PI=4*ATN(1): NN=1: NV=1: LN=0: LV=10: LH=2: AM1=4: AM2=4
 Z1=2: Z2=2: A1=41.4686: PM=AM1*AM2/(AM1+AM2): B1=2*PM/A1
 AK=1.439975*Z1*Z2*B1: N=2000: R00=20: HH=R00/N
 REM *************** AL - AL 51.1 ******************
 E1(1)=51.1
REM ********** THE PHASE SHIFTS AL - AL 51.1 ***************
 FR(0)=291: FR(2)=245: FR(4)=163: FR(6)=28: FR(8)=4.2: FR(10)=0.5
 FM(0)=0.51: FM(2)=0.51: FM(4)=0.53: FM(6)=0.855: FM(8)=0.985
 FM(10)=0.998: FOR I=NN TO NV: E(I)=E1(I)*PM/AM1: NEXT I
 FOR I=LN TO LV STEP LH: FR1(I)=FR(I)*PI/180
 REM FM1(I)=FM(I)*PI/180
NEXT I: REM ********* THE  INITIAL PARAMETERS  ********
 V22=122: A22=0.74: R22=1.81: V33=11: A33=0.74: R33=1.81
 RCU=1.81: VN2=-V22*B1: VN3=-V33*B1
REM  ** CALCULATION OF THE SCATTERING  PHASE SHIFTS **
 FOR JJ=NN TO NV: SK=E(JJ)*B1: SS=SQR(SK)
 GG=3.44476E-02*Z1*Z2*PM/SS: SIGMRR=0: SIGMAS=0
 FOR L=LN TO LV STEP LH
 CALL FUN (X(), Y(),  R22, VN2, A22, R33, VN3, A33, RCU, L, SK,
AK)
```

```
 RR1=HH*SS*(N-5): RR2=HH*SS*N: X1=X(N-5): X2=X(N)
 Y1=Y(N-5): Y2=Y(N)
REM *********  THE COULOMB FUNCTIONS ********
 CALL CUL(GG,RR1,L,F1,G1,FP1,GP1)
 CALL CUL(GG,RR2,L,F2,G2,FP2,GP2)
REM ********** THE SEARCH OF PHASE SHIFTS *********
 AA1=X2*F1-X1*F2: BB1=Y1*G2-Y2*G1: DD1=X1*G2-X2*G1
 CC1=Y2*F1-Y1*F2: AA=BB1-AA1: BB=-CC1-DD1: CC=AA1+BB1
 DD=CC1-DD1: DD0=AA^2+BB^2: SS1=(AA*CC+BB*DD)/DD0
 SS2=(AA*DD-BB*CC)/DD0: ETA(JJ,L)=SQR(SS1^2+SS2^2)
 SS22=SS2/ETA(JJ,L): SS11=SS1/ETA(JJ,L)
 SIG(JJ,L)=-LOG((ETA(JJ,L)))/2
 FAZ=SS22/(1+SS11): FAZ(JJ,L)=ATN(FAZ): IF FAZ(JJ,L)>0 GOTO
901
 FAZ(JJ,L)=FAZ(JJ,L)+PI
901 FAZA(JJ,L)=FAZ(JJ,L)*180/PI: IF SIG(JJ,L)>0 GOTO 911
 SIG(JJ,L)=SIG(JJ,L)+PI
911 SIG(JJ,L)=SIG(JJ,L)*180/PI: A=FAZ(JJ,L)
 SIGMAR = SIGMAR + (2*L+1)*(1 - (ETA(JJ,L))^2)
 SIGMAS = SIGMAS + (2*L+1)*(ETA(JJ,L))^2*(SIN(A))^2
PRINT USING " +#.###^^^^ "; L; FR(L); FAZA(JJ,L); FM(L); SIG(JJ,L)
 ETA(JJ,L): NEXT L: SIGMAR=10*4*PI*SIGMAR/SK
 SIGMAS=10*4*PI*SIGMAS/SK
 PRINT "       SIGR - THEOR = ";SIGMAR;
 PRINT "       SIGS - THEOR = ";SIGMAS: NEXT JJ
REM ******* THE CALCULATION OF DIF. CROSS SECTIONS *****

 FOR J=NN TO NV: SK=E(J)*B1: SS=SQR(SK)
 GG=3.44476E-02*Z1*Z2*PM/SS: SIGMAR=0: SIGMAS=0
 FOR L=LN TO LV STEP LH: A=FR1(L): ET(L)=FM(L)
 SIGMAR = SIGMAR + (2*L+1)*(1 - (ET(JJ,L))^2)
 SIGMAS = SIGMAS + (2*L+1)*(ET(JJ,L))^2*(SIN(A))^2: NEXT L
 SIGMAR=10*4*PI*SIGMAR/SK: SIGMAS=10*4*PI*SIGMAS/SK
 PRINT "       SIGR - EXP = ";SIGMAR;
 PRINT "       SIGS - EXP = ";SIGMAS
 NEXT J: TMI=10: TMA=90: TH=1
```

```
 CALL SEC (FR1(), GG, SS, TMI, TMA, TH, SEC(), ET(), LN, LV, LH,
1)
 FOR T=TMI TO TMA/3 STEP TH
 PRINT USING " ####.##  "; T; SEC(T); T+20; SEC(T+20); T+40;
SEC(T+40); T+60; SEC(T+60): NEXT
REM ************** FILE RECORDING ************
 IF SAVE=0 THEN STOP: OPEN "O",1,G$
 PRINT#1, "ALPHA-ALPHA FOR LAB E=";: PRINT#1, E1(NN)
 FOR T=TMI TO TMA STEP TH: PRINT#1, USING " #.###^^^^
";T;SEC(T)
 NEXT
END

SUB CUL(GG,RR2,L,F2,G2,FP2,GP2)
 Q=GG: R=RR2: F0=1: GK=Q*Q: GR=Q*R: RK=R*R
 B01=(L+1)/R+Q/(L+1): K=1: BK=(2*L+3)*((L+1)*(L+2)+GR)
 AK=-R*((L+1)^2+GK)/(L+1)*(L+2)
 DK=1/BK: DEHK=AK*DK: S=B01+DEHK
112 K=K+1: AK=-RK*((L+K)^2-1)*((L+K)^2+GK)
 BK=(2*L+2*K+1)*((L+K)*(L+K+1)+GR): DK=1/(DK*AK+BK)
 IF DK>0 GOTO 132: F0=-F0
132 DEHK=(BK*DK-1)*DEHK: S=S+DEHK
 IF (ABS(DEHK)-1E-10)>0 GOTO 112: FL=S: K=1: RMG=R-Q
 LL=L*(L+1): CK=-GK-LL: DK=Q: GKK=2*RMG: HK=2
 AA1=GKK*GKK+HK*HK: PBK=GKK/AA1: RBK=-HK/AA1
 OMEK=CK*PBK-DK*RBK: EPSK=CK*RBK+DK*PBK
 PB=RMG+OMEK: QB=EPSK
152 K=K+1: CK=-GK-LL+K*(K-1): DK=Q*(2*K-1): HK=2*K
 FI=CK*PBK-DK*RBK+GKK: PSI=PBK*DK+RBK*CK+HK
 AA2=FI*FI+PSI*PSI: PBK=FI/AA2: RBK=-PSI/AA2
 VK=GKK*PBK-HK*RBK: WK=GKK*RBK+HK*PBK: OM=OMEK
 EPK=EPSK: OMEK=VK*OM-WK*EPK-OM
 EPSK=VK*EPK+WK*OM-EPK
 PB=PB+OMEK: QB=QB+EPSK
 IF (ABS(OMEK)+ABS(EPSK)-1E-10)>0 GOTO 152: PL=-QB/R
 QL=PB/R: G0=(FL-PL)*F0/QL: G0P=(PL*(FL-PL)/QL-QL)*F0
```

```
F0P=FL*F0: ALFA=1/(SQR(ABS(F0P*G0-F0*G0P))): G2=ALFA*G0
GP2=ALFA*G0P: F2=ALFA*F0: FP2=ALFA*F0P
W=1-FP2*G2+F2*GP2
END SUB

SUB FUN(X(5000), Y(5000), R2, V2, A2, R3, V3, A3, RCU, L, SK,
AK)
SHARED HH,N:  HK=HH*HH: X(0)=0: X(1)=1E-3: Y(0)=0: Y(1)=1E-3
FOR K=1 TO N-1: R=K*HH: FR1=V2/(1+EXP((R-R2)/A2))
FC1=V3/(1+EXP((R-R3)/A3)): FR=SK-FR1-L*(L+1)/R^2
IF R>RCU GOTO 177: FR=FR-AK/(2*RCU)*(3-(R/RCU)^2): GOTO
188
177 FR=FR-AK/R
188 FC=FC1: F=2-FR*HK: G=FC*HK: X(K+1)=F*X(K)-X(K-1)-G*Y(K)
Y(K+1)=F*Y(K)-Y(K-1)+G*X(K): NEXT
END SUB

SUB SEC (F(100), GG, SS, TMI, TMA, TH, S(100), E(100), LMI,
LMA, LH, NYS)
SHARED PI: DIM S0(20),P(20)
RECUL1=0: AIMCUL1=0: CALL CULFAZ(GG,S0())
FOR TT=TMI TO TMA STEP TH: T=TT*PI/180: XP=COS(T)
A=2/(1-XP): BB=-GG*A: ALO=GG*LOG(A)+2*S0(0)
RECUL=BB*COS(ALO): AIMCUL=BB*SIN(ALO)
IF NYS=0 GOTO 555
PT=PI-T: X1P=COS(PT): A1=2/(1-X1P): BB1=-GG*A1
ALO1=GG*LOG(A)+2*S0(0): RECUL1=BB1*COS(ALO1)
AIMCUL1=BB1*SIN(ALO1)
555 RENUC=0: AIMNUC=0: RENUC1=0: AIMNUC1=0
FOR L=LMI TO LMA STEP LH: AL=E(L)*COS(2*F(L))-1
BE=E(L)*SIN(2*F(L)): LL=2*L+1: SL=2*S0(L)
CALL POLLEG(XP,L,P())
RENUC=RENUC+LL*(BE*COS(SL)+AL*SIN(SL))*P(L)
AIMNUC=AIMNUC+LL*(BE*SIN(SL)-AL*COS(SL))*P(L)
IF NYS=0 GOTO 556: CALL POLLEG(X1P,L,P())
RENUC1=RENUC+LL*(BE*COS(SL)+AL*SIN(SL))*P(L)
```

```
AIMNUC1=AIMNUC+LL*(BE*SIN(SL)-AL*COS(SL))*P(L)
556 NEXT L: RE=RECUL+RECUL1+RENUC+RENUC1
AIM=AIMCUL+AIMCUL1+AIMNUC+AIMNUC1
S(TT)=10*(RE^2+AIM^2)/4/SS^2: NEXT TT: END SUB
SUB POLLEG(X,L,P(20))
P(0)=1: P(1)=X: FOR I=2 TO L: P(I)=(2*I-1)*X/I*P(I-1)-(I-1)/I*P(I-2)
NEXT
END SUB

SUB CULFAZ(G,F(20))
C=0.577215665: S=0: N=50: A1=1.202056903/3: A2=1.036927755/5
FOR I=1 TO N: A=G/I-ATN(G/I)-(G/I)^3/3+(G/I)^5/5
S=S+A: NEXT: FAZ=-C*G+A1*G^3-A2*G^5+S: F(0)=FAZ
FOR I=1 TO 20: F(I)=F(I-1)+ATN(G/(I)): NEXT
END SUB
```

We will provide the results of the control account by this program. The real physical scattering process in the $^4He^4He$ system of nuclear particles was considered at energy of 51.1 MeV with a complex potential. Experimental data on differential cross sections are given in [62]. The analysis of these data in the optical model was carried out in the same paper. Consequently, parameters of the Woods-Saxon potential were found

$$V(r) = \frac{V + iW}{\left[\exp\left(\frac{r-R}{a}\right)+1\right]} + V_c(r), \qquad (1.4.1)$$

where $V_c(r)$ – The Coulomb potential and

$V = -122 \pm 3$ MeV, $W = -11 \pm 2$ MeV,

$R = 1.81$ fm, $a = 0.74 \pm 0.03$ fm, $R_c = R$.

Such potential leads to the scattering phase shifts and parameters of the inelasticity, which are given in tab. 1.4.1. Also the total experimental cross section of the reaction $\sigma_r = 770 \pm 100$ mb is given in work [62] at this

energy.

Tab. 1.4.1 - Results of the phase shift analysis.

L	δ, degree, [62]	δ, degree, (Our calculation)	η [62]	η (Our calculation)
0	111±4	1.123E+02	0.51±0.07	5.102E-01
2	65±4	6.655E+01	0.51±0.07	5.177E-01
4	163±4	1.649E+02	0.53±0.07	5.414E-01
6	28±3	2.935E+01	0.855±0.03	8.501E-01
8	4.2±0.6	4.422E+00	0.985±0.004	9.841E-01
10	0.5±0.1	7.464E -01	0.998±0.001	9.972E-01

Using these parameters of the potential, the calculations of the scattering phase shifts given in tab. 1.4.1 and the total cross section of the reactions of $\sigma_r = 766.1$ mb have been executed according to the program given above. It is clear that practically all calculated values (excepting the last real phase shift for $L = 10$), within the errors, coincide with the results [62]. If to use the phase shifts [62], then for the cross section of reactions turns out the value $\sigma_r = 764.7$ mb, which also as well as previously, will well be coordinated with the experimental data.

Thus, in the case of the real central potentials, the general and numerical methods of the solution of one Schrödinger equation are considered, the accuracy of the physical calculations, which allow one to obtain such methods and their full applicability for finding of the nuclear scattering phase shifts is shown. The control calculations of the nuclear scattering phase shifts of the various nuclear particles by the finite-difference method and by the Runge-Kutt method with the real interaction potentials are executed and mutual comparison, which shows the coincidence of the results to the accuracy of an order of the several 100-th shares of percent is carried out.

The case when the central potential contains, both real, and imaginary parts is considered. Then the Schrödinger equation passes into the coupled equation system. The general and numerical methods of the solution of such system with rather simple initial and asymptotic conditions are stated.

For this case the control calculations of the nuclear scattering phase shifts and their comparison with some results obtained in other works are also given.

1.5 Creation of the intercluster potentials

We will stop in more detail on the procedure of the construction of the intercluster partial potentials at the given orbital moment L, having defined the criteria and sequence of finding of the parameters and having specified their errors and ambiguities. First of all there are parameters of BS potentials, which at the given number of the states allowed and forbidden in this partial wave are fixed quite unambiguously on the binding energy, radius of nucleus and an asymptotic constant in the considered channel.

The accuracy, on which thus parameters of the BS potential are determined, is connected, first of all, with the AC accuracy, which usually makes 10–20%. The accuracy of the experimental determination of the charge radius usually is much higher than 3–5%. Such potential does not contain other ambiguities as the classification of states according to Young tableaux allows one to fix unambiguously number of the BS, forbidden or allowed states in this partial wave, which completely determines its depth and potential width entirely depends on the value of the AC. The principles of the determination of number of the FS and AS are given in the given partial wave, for example, in [2].

Here it is necessary to notice that the calculations of the charge radius in any model contain the model errors, i.e. errors which are caused by the accuracy of the model itself. In any model the values of such radius depend on the integral from the model WF, i.e. the model errors of such functions are just summarized. The values of the AC are determined by an asymptotics of the model of the WF in one point on their asymptotics and, apparently, contain significantly smaller error. Therefore, generally BS potentials have to be constructed so first of all as much as possible to be coordinated with the values of the AC obtained on the basis of the independent methods, which allow one to take the AC from the experimental data [63].

Intercluster potential of the non-resonance scattering process on the phase shifts at the given number of the BS, allowed and forbidden states in the considered partial wave, is also constructed quite unambiguously. The accuracy of the determination of the parameters of such potential is connected, first of all, with the accuracy of extraction of the phase shifts from the experimental data and can reach 20–30%. Here, such potential

does not contain the ambiguities as the classification of states according to Young tableaux allows one to fix unambiguously the number BS, which completely determines its depth, and potential width with the given depth is defined by a form of this phase shift.

At the creation of the non-resonance scattering potential according to the data of the spectra of nucleus in a certain channel, it is difficult to estimate the accuracy of finding of its parameters even at the given number of the BS though it is possible to hope, apparently, that it not much more exceeds an error in the previous case. Such potential is as usual supposed for the area of energies up to 1 MeV, has to lead to the phase shift closing to zero or give smoothly falling down phase shift form as in the spectra of nucleus there are no resonance levels.

In the analysis of the resonance scattering, when at the considered partial wave at the energies to 1 MeV there is the rather narrow resonance with a width about 10–50 keV, at the given number of BS, the potential is also constructed completely unambiguously. At the given number of BS its depth is unambiguously fixed by the resonance energy of the level, and the width is completely defined by the width of such resonance. The error of its parameters usually does not exceed an error of the determination of the width of such level and makes about 3–5%. Meanwhile, this also applies to the construction of the partial potential by the phase shifts and determination of its parameters by a resonance in the spectra of nucleus.

As a result, all potentials do not contain the ambiguities and allow one to describe correctly the total cross sections of the processes of the radiative capture [2,28] without the obvious involvement of such concept as the spectroscopic S_f factor, i.e. its value just is accepted equal to the unit as it has been used in work [64]. In other words, by the consideration of the capture reaction in the modified PCM [2] for the potentials of the processes correlated in a continuous spectrum with the characteristics of the scattering processes and a discrete spectrum describing the main properties of the BS of nucleus coordinated in a continuous spectrum with characteristics it is not required to enter an additional multiplier S_f [64] any more. Apparently, all effects present in reaction, including the probability of a cluster configuration, are considered at the creation of the interaction potentials.

It is possible because the potentials are constructed taking into account

the structure of the FS and on the basis of the description of observed, i.e. the experimental characteristics of the interacting clusters in the initial channel and some nucleus formed in final state in case of the description by its cluster design consisting of the initial particles. Thereby, the presence of S_f taking into account in the wave functions of the BS clusters, defined on the basis of such potentials in case of the solution of Schrödinger equation (1.1.1).

In conclusion we will note that in case of the creation of partial interaction potentials it is considered that they depend not only on the L orbital moment, but also on the S total spin and the J total moment of the cluster system. In other words, for the different moments L,S,J we will have the different values of the parameters. As usually the $E1$ or $M1$ transitions between the different states $^{(2S+1)}L_J$ in continuous and discrete spectra are considered, then the potentials of these states will be various.

1.6 Potentials and wave functions

The intercluster interaction potentials for each partial wave, i.e. for the given orbital moment L, and the pointlike Coulomb member can be chosen in the form

$$V(r) = V_0\exp(-\gamma r^2) + V_1\exp(-\delta r^2) \qquad (1.6.1)$$

or

$$V(r) = V_0\exp(-\gamma r^2). \qquad (1.6.2)$$

Here the parameters V_0 and V_1, γ and δ are potential parameters, which usually are from a condition of the best description of the phase shifts of elastic scattering taken in the course of the phase shift analysis from the experimental data by the differential cross sections, i.e. angular distributions or excitation functions.

The coulomb potential at the zero Coulomb radius of $R_{coul} = 0$ written in the form

$$V_{coul}(\text{МэВ}) = 1.439975 \cdot \frac{Z_1 Z_2}{r},$$

where r – relative distance between the particles of the initial channel in fm and Z – charges of particles in terms of an elementary charge "e".

The behavior of the wave function of the bound states, including, the ground states of the nucleus in the cluster channels at long distances is characterized by the asymptotic constant C_w, which is defined by the Whittaker's function [65]

$$\chi_L(r) = \sqrt{2k_0}C_w W_{-\eta L+1/2}(2k_0 r), \qquad (1.6.3)$$

where $\chi_L(R)$ – the numerical wave function of the bound state obtained from the solution of the radial Schrödinger equation and normalized on the unit, $W_{-\eta L+1/2}$ – Whittaker's function of the bound state defining the

asymptotic behavior of the WF and being the solution of the same equation without nuclear potential, i.e. at long distances R, k_0 – the wave number caused by the channel binding energy, η – the Coulomb parameter determined further and L – the orbital moment of the bound state.

The asymptotic constant is the important nuclear characteristic defining the behavior of the "tail", i.e. an asymptotics of the wave function at long distances. In many cases its knowledge for A nucleus in the cluster channel $b+c$ defines the value of an astrophysical S-factor for the process of the radiative captures of $b(c,\gamma)A$ [63]. The asymptotic constant is proportional to nuclear vertex constant for the virtual process of $A \rightarrow b+c$, which is a matrix element of this process on the mass surface [66].

1.7 Methods of the phase shift analysis

Knowing the experimental differential cross sections of the elastic scattering it is always possible to find some set of the parameters called the phase shifts $\delta^J_{S,L}$, allowing one to describe the behavior of these cross sections with certain accuracy. The quality of the description of the experimental data on the basis of some theoretical function (a functionality of several variables) can be estimated by the χ^2 method, which is presented in the form [6]

$$\chi^2 = \frac{1}{N}\sum_{i=1}^{N}\left[\frac{\sigma_i^t(\theta)-\sigma_i^e(\theta)}{\Delta\sigma_i^e(\theta)}\right]^2 = \frac{1}{N}\sum_{i=1}^{N}\chi_i^2, \qquad (1.7.1)$$

where σ^e and σ^t – the experimental and theoretical, i.e. calculated at some given values of phase shifts $\delta^J_{S,L}$ cross section of the elastic scattering of the nuclear particles for the i scattering angle, $\Delta\sigma^e$ – an error of the experimental cross sections for this angle and N – number of experimental measurements.

The expressions, describing the differential cross sections are the decomposition of some functionality $d\sigma(\theta)/d\Omega$ in the numerical series [6], and it is necessary to find such variation parameters of decomposition $\delta^J_{S,L}$, which in the best way describe its behavior. As the expressions for the differential cross sections usually are exact [6], at the increase in members of the decomposition of L to the indefinitely the value χ^2 has to aspire to zero. This criterion was used for the choice of the certain set of phase shifts leading to a minimum χ^2, which could apply for a role of a global minimum of this multiple parameter variation problem [5]. In more detail the methods and criteria of the phase shift analysis used in these calculations are given in works [5,10].

Thus, for the search of the scattering phase shifts according to the experimental cross sections the procedure of minimization of χ^2 functionality (1.7.1) as the functions of a certain number of variables, was executed, each of which is a $\delta^J_{S,L}$ phase shift of some partial wave. For the solution of this problem there is minimum χ^2 in some limited area of values

of these variables is looked for. But also it is possible to find a set of local minima χ^2 with the unit order value in this area. The choice of the smallest of them allows one to hope that it will correspond to a global minimum, which is the solution of such variation problem.

The stated criteria and methods were used by us for the carrying out of the phase shift analysis at low energies, which is important for the majority of the astrophysical problems. All expressions for the calculation of the differential cross sections of the elastic scattering of particles with the different spins, which are required for carrying out of the phase shift analysis in the systems stated above, are given further in the corresponding paragraphs of chapter 2.

1.8 General principles of the three-body model

We will consider the radial Schrödinger equation with the central nuclear forces for the wave function of the system of three particles [67,68]

$$(H - E)\Phi_{l,\lambda}(r,R) = 0. \qquad (1.8.1)$$

where

$$H = T + V,$$

$$T = T_1 + T_2 = -\frac{\hbar^2}{2\mu}\Delta_r - \frac{\hbar^2}{2\mu_0}\Delta_R, \qquad (1.8.2)$$

$$V = V_{12} + V_{23} + V_{13},$$

$$\mu = \frac{m_2 m_3}{m_{23}}, \quad \mu_0 = \frac{m_1 m_{23}}{m},$$

$$m_{23} = m_2 + m_3, \quad m = m_1 + m_2 + m_3.$$

Here m and μ – the masses and the reduced mass of three particles, Δ – Laplasian operator on two coordinates of r and R, T and V – operators of the kinetic and potential energy, H – complete Hamiltonian of a system and E – energy of system, i.e. eigenvalues of energy in this system for the given Hamiltonian.

The r value in such record defines the distance between particles 2 and 3, which are in the triangle basis from three bodies with the orbital moment λ, and R is a distance between the first particle, which is located in top of a triangle and the center of mass of the first two particles with the orbital moment l.

Total three-body wave function of such system has the form [67]

$$\Psi(r,R) = \sum_{l,\lambda} \Phi_{l,\lambda}(r,R) Y_{LS}^{JM}(\hat{r},\hat{R}),$$

and its angular part $Y_{LS}^{JM}(\hat{r},\hat{R})$ is written in a usual form [69,70,71]

$$Y_{LS}^{JM}(\hat{r},\hat{R}) = \sum_{M_S M_L} \langle LM_L SM_S | JM \rangle Y_{LM_L}(\hat{r},\hat{R}) \chi_{SM_s}(\sigma).$$

Here $\boldsymbol{L} = \boldsymbol{l} + \boldsymbol{\lambda}$ – the total orbital moment, S – total spin of the system, J – the total moment of the considered system of particles, M – projections of these moments, $Y_{LS}^{JM}(\hat{r},\hat{R})$ – spin-angular function [69-71], $\Phi_{l,\lambda}$ – the radial wave function, which is usually written down in the form

$$\Phi_{l,\lambda}(r,R) = Nr^{\lambda}R^{l}\sum_i C_i \exp(-\alpha_i r^2 - \beta_i R^2) = N\sum_i C_i \Phi_i, \qquad (1.8.3)$$

r and R – scalar distances between particles, $\hat{r}$ and $\hat{R}$ – angles between the directions of vectors of $\boldsymbol{r}$ and $\boldsymbol{R}$ and an axis z, Y_{LM} – spherical function [72], χ_{SM} – the spin function of system depending on a σ spin of the particles, angular brackets designate the Clebsch-Gordan coefficients [72].

The actual calculations for certain values of the variational parameters α_i and β_i (1.8.3) we find the energy of the system, which gives the zero determinant of the system (1.8.1), and then, by varying these parameters, searches for a minimum of energy. On the following step we increase the dimension of the N basis and repeat all calculations until the size of eigenvalue, i.e. the binding energy E_N, on the next step of N does not begin differ from the previous E_{N-1} value at a size ε, which is usually set at the level of 0.1–1.0%. According to the general variation principles [9] this minimum energy will also be real three-body binding energy of the system, i.e. the binding energy of an atomic nucleus in the cluster model considered here.

1.9 Variation methods of three-body model

The matrix elements of the system Hamiltonian (1.8.2) and overload integrals calculated on the basic of Φ_i (1.8.3) functions have the form [73]

$$T_{ij} = \frac{\pi}{16} N^2 \frac{\hbar^2}{m_N} \frac{(2l+1)!!(2\lambda+1)!!}{2^{l+\lambda}} \alpha_{ij}^{-\lambda-1/2} \beta_{ij}^{-l-1/2} G_{ij},$$

$$G_{ij} = \frac{B_{ij}(\alpha,\lambda)}{\mu\beta_{ij}} + \frac{B_{ij}(\beta,l)}{\mu_0\alpha_{ij}}, \qquad B_{ij}(\delta,\nu) = \frac{\nu^2}{2\nu+1} + \frac{\delta_i\delta_j}{\delta_{ij}^2}(2\nu+3) - \nu,$$

$$L_{ij} = \frac{\pi}{16} N^2 \frac{(2l+1)!!(2\lambda+1)!!}{2^{l+\lambda}} \alpha_{ij}^{-\lambda-3/2} \beta_{ij}^{-l-3/2}, \qquad N = \left(\sum_{ij} C_i C_j L_{ij} \right)^{-1/2},$$

with the potentials (designations are used here: cb – centrifugal, coul – Coulomb)

$$[(V_{cb})_R]_{ij} = \frac{\pi}{16} N^2 \frac{\hbar^2}{\mu_0} l(l+1) \frac{(2l-1)!!(2\lambda+1)!!}{2^{l+\lambda}} \alpha_{ij}^{-\lambda-3/2} \beta_{ij}^{-l-1/2},$$

$$[(V_{cb})_r]_{ij} = \frac{\pi}{16} N^2 \frac{\hbar^2}{\mu} \lambda(\lambda+1) \frac{(2\lambda-1)!!(2l+1)!!}{2^{l+\lambda}} \alpha_{ij}^{-\lambda-1/2} \beta_{ij}^{-l-3/2},$$

$$[\{V_{coul}(23)\}_r]_{ij} = Z_2 Z_3 \frac{\pi}{16} N^2 \frac{2}{\sqrt{\pi}} \frac{(2l+1)!!}{2^l} \frac{\lambda!}{\alpha_{ij}^{\lambda+1} \beta_{ij}^{l+3/2}},$$

$$[\{V_{coul}(12)\}_R]_{ij} = Z_1 Z_2 \frac{\pi}{16} N^2 \frac{2}{\sqrt{\pi}} \frac{(2\lambda+1)!!}{2^\lambda} \frac{l!}{\beta_{ij}^{l+1} \alpha_{ij}^{\lambda+3/2}},$$

$$[\{V_{coul}(13)\}_R]_{ij} = Z_1 Z_3 \frac{\pi}{16} N^2 \frac{2}{\sqrt{\pi}} \frac{(2\lambda+1)!!}{2^\lambda} \frac{l!}{\beta_{ij}^{l+1} \alpha_{ij}^{\lambda+3/2}},$$

$$(V_{23})_{ij} = \frac{\pi}{16} N^2 V_{23} \frac{(2l+1)!!(2\lambda+1)!!}{2^{l+\lambda}} (\alpha_{ij} + \gamma_{23})^{-\lambda-3/2} \beta_{ij}^{-l-3/2},$$

$\alpha_{ij} = \alpha_i + \alpha_j, \qquad \beta_{ij} = \beta_i + \beta_j.$

Furthermore, for example, at values $l = 1$ and $\lambda = 0$ we have the following expressions for the matrix elements from the nuclear potentials of the form (1.6.2)

$$(V_{12})_{ij} = \frac{\pi}{16} N^2 \frac{3V_{12}}{2A_{ij}^{3/2}(\beta_{ij} + \gamma_{12})} \left[\frac{a^2\gamma_{12}^2}{A_{ij}} + 1 \right],$$

where

$$A_{ij} = \alpha_{ij}\beta_{ij} + \gamma_{12}(\alpha_{ij} + a^2\beta_{ij}) \ , \quad a = m_3 / m_{23} \ .$$

In the case of $l = 0$ and $\lambda = 0$ for this part of potential we find the expression

$$(V_{12})_{ij} = \frac{\pi}{16} N^2 \frac{V_{12}}{A_{ij}^{3/2}}.$$

Here the value γ_{12} is the parameter of the width of Gaussian potential, and V_{12} – its depth between the corresponding couple of particles, in this case, 12 or 13.

For a case of any l when $\lambda = 0$ it is possible to obtain the expression

$$(V_{12})_{ij} = \frac{\pi}{16} N^2 V_{12} \frac{(2l+1)!!}{2^l} \frac{d_{ij}^l}{A_{ij}^{l+3/2}} \ ,$$

where

$$d = \alpha_{ij} + \gamma_{12}a^2.$$

The mean square mass radius of a nucleus in such model is presented in the form [74]

$$< r^2 >_m = m_1 / m < r^2 >_{m1} + m_2 / m < r^2 >_{m2} + m_3 / m < r^2 >_{m3} + A / m$$

$$A = \frac{\pi}{16} N^2 \frac{(2l+1)!!(2\lambda+1)!!}{2^{l+\lambda+1}} \sum_{ij} C_i C_j \alpha_{ij}^{-\lambda-3/2} \beta_{ij}^{-l-3/2} \left(\frac{2\lambda+3}{\alpha_{ij}} \mu + \frac{2l+3}{\beta_{ij}} \mu_0 \right)$$

$$\mu = \frac{m_2 m_3}{m_{23}}, \quad \mu_0 = \frac{m_1 m_{23}}{m}, \quad m_{23} = m_2 + m_3, \quad m = m_1 + m_2 + m_3 \quad .$$

The mean square charge radius of a nucleus in the three-body model has the form

$$< r^2 >_z = Z_1 / Z < r^2 >_{z1} + Z_2 / Z < r^2 >_{z2} + Z_3 / Z < r^2 >_{z3} + B / Z$$

Here the value B is expressed through the moments of particles, variation parameters and coefficients of decomposition of the WF as follows:

$$B = \frac{\pi}{16} N^2 \frac{(2l+1)!!(2\lambda+1)!!}{2^{l+\lambda+1}} \sum_{ij} C_i C_j \alpha_{ij}^{-\lambda-3/2} \beta_{ij}^{-l-3/2} \left(\frac{2l+3}{\beta_{ij}} C + \frac{2\lambda+3}{\alpha_{ij}} D \right) +$$

$$+ N^2 E (\lambda+1)! (l+1)! \sum_{ij} \frac{C_i C_j}{2\alpha_{ij}^{\lambda+2} \beta_{ij}^{l+2}} ,$$

$$C = \frac{Z_1 m_{23}^2 + Z_{23} m_1^2}{m^2} , \qquad Z_{23} = Z_2 + Z_3 ,$$

$$D = \frac{Z_2 m_3^2 + Z_3 m_2^2}{m_{23}^2} ,$$

$$E = \frac{m_1}{m m_{23}} (Z_3 m_2 - Z_2 m_3) .$$

As the charge and mass radiuses of the clusters, namely, a proton, a deuteron, a triton, helium-3 and α particles if they are not brought in the appropriate chapter in addition, values were accepted as $\langle r\rangle_{zn} = 0$ fm, $\langle r\rangle_{mn} = \langle r\rangle_{mp} = \langle r\rangle_{zp} = 0.877$ fm, $\langle r\rangle_{md} = \langle r\rangle_{zd} = 1.96$ fm, $\langle r\rangle_{mt} = \langle r\rangle_{zt} = 1.72$ fm, $\langle r\rangle_{m3He} = \langle r\rangle_{z3He} = 1.88$ fm, $\langle r\rangle_{m\alpha} = \langle r\rangle_{z\alpha} = 1.67$ fm [75,76,77,78].

At the search of the binding energy of a nucleus in the three-body model the initial values of the variation α_i and β_i parameters were found from a linear grid of the form

$$\alpha_i = i/30, \quad \beta_i = 2\alpha_i.$$

Then the independent variation of each of these parameters at the given number of iterations was carried out so that to minimize the energy of the system with the given accuracy ε. This variation method differs a little from the similar variant of the VM from the usual two-body problem [28,79,80].

To check the variation three-body method of calculation and the computer program considered above the model problem for three particles interacting in the Afnan-Tang potential [81] with the averaging the triplet and the singlet states was used. For the binding energy of such system in work [81] value of -7.74 MeV is obtained, and the value -7.76 MeV was found in articles [82], where the non-orthogonal variation method with the change of the α and β parameters of wave function on the basis of a tangential grid was used. We, on the basis of the methods stated above, at an independent variation of all parameters and dimension basis $N = 5$, have obtained -7.83 MeV. Thereby, the binding energy of the model system considered here obtained on the basis of the methods described above has changed approximately for 1% concerning results of works [81,82] that it is possible to consider as quite good consent.

Conclusion

Thus, all main mathematical expressions and some programs for searching of the elastic scattering phase shifts and calculations of nuclear characteristics are given in the three-body model. The description of the alternative methods of the search of eigenvalues for two- or three-body generalized variation problem is included. Such method leads to the steadier numerical scheme of the variation solution of the Schrödinger equation in comparison with usual methods of orthogonalization according to Schmidt.

The criteria of creation of two-partial potentials on the basis of the scattering phase shifts and the general principles for search of such phase shifts at carrying out of the phase shift analysis are defined. The several ways of the calculation of values of wave function applicable both for a scattering problem, and for a discrete spectrum are described. The finite-difference and variation methods of search the binding energy of nuclear system, based on two- and three-partial models, are given.

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AUTHOR INFORMATION

Dubovichenko Sergey Borisovich - Laureate of the al-Farabi State Prize of the Republic of Kazakhstan (RK) in the field of science and technology; doctor of physical and mathematical sciences (on specialties 01.04.16 - physics of an atomic nucleus and elementary particles and 05.13.18 - mathematical modeling, numerical methods and complexes of programs) in the RK and the Russian Federation (RF), professor RK;

vice-president and academician of the European Academy of Natural Sciences (EU), academician of the Peter's Academy of Sciences and Arts (RF), academician of the Russian Academy of Natural History (RF), academician of the International Academy of Informatization (RK), academician of the New York Academy of Sciences (US);

member of the International Astronomical Union (IAU); member of the American Physical Society (US), member of the European Physical Society (EU);

laureate of the European Gold Medal, Gauss Medal and Honorary Cross "Merit";

laureate of the State Scientific Stipend of RK, laureate of the International Soros Grant, laureate of the Komsomol Prize of Kaz.SSR 1984 (in former USSR);

chief of Kazakhstan department (www.eans.kz) of European Academy of Natural sciences (www.eanw.org) in the field of physics and astrophysics;

head of the laboratory "Nuclear astrophysics" at Fesenkov Astrophysical Institute of the National Center of Space Researches and Technologies of Aerospace Agency of Ministry Defense and Aerospace Industry of RK.

E-mail: dubovichenko@mail.ru , dubovichenko@gmail.com

Web-site: www.dubovichenko.ru

Fesenkov Astrophysical Institute - Observatory 23, Kamenskoe plato, 050020, Almaty, Republic of Kazakhstan, www.aphi.kz